PSEUDOSPECTRAL METHODS WITH VARIOUS BASIS FUNCTIONS AND APPLICATIONS TO QUANTUM MECHANICS

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This is to certify that we have read the thesis PSEUDOSPECTRAL METHODS WITH VARIOUS BASIS FUNCTIONS AND APPLICATIONS TO QUANTUM MECHANICS submitted by SAEIDA WLIE 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 WITH VARIOUS BASIS FUNCTIONS AND APPLICATIONS TO QUANTUM MECHANICS

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In this thesis, we studied the pseudospectral methods and their application to the solution of eigenvalue problems associated with ordinary differential equations. In particular, we considered second order differential equations and a specific example, the Schrödinger equation for quantum dynamical systems with polynomial potentials.

After an introduction to self adjoint eigenvalue problems and the Schrödinger equation for particles, in the presence of polynomial potentials, we recollected some important properties of Lagrange interpolation and orthogonal polynomials. We presented a method to compute the zeros of an orthogonal polynomial of arbitrary degree by means of a symmetric tridiagonal matrix eigenvalue problem. We constructed the particular symmetric tridiagonal matrices for computation of the zeros of Hermite, Associated Laguerre, Chebyshev and Legendre polynomials.

After that, we explained in details the pseudospectral schemes using Hermite and Associated Laguerre polynomials by studying some published articles. We also made substitutions on the independent variable in order to transform infinite interval to a finite one and derived pseudospectral formulations using Chebyshev and Legendre polynomials.

As a specific example, we applied the pseudospectral methods using the four types of orthogonal polynomials mentioned above to the Schrödinger equation for quantum dynamical systems with polynomial potentials. We compared our numerical results with the numerical results obtained previously by other authors and made comments about the efficiency of our method.

Keywords: Schrödinger equation, orthogonal polynomials, self-adjoint eigenvalue problems.

ÖZ

ÇEŞİTLİ TABAN FONKFİYONLARI İLE SANKİ-SPEKTRAL YÖNTEMLER VE KUVANTUM MEKANİĞE UYGULAMALARI

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Bu çalışmada, sanki-spektral yöntemler ve onların sıradan difereansiyel denklemler ile ilgili özdeğer problemlere uygulamalarını inceledik. Özel olarak, ikinci mertebeden diferansiyel denklemleri ve belirli örnek olarak polinom potansiyelli kuvantum sistemlerin Schrödinger denklemini ele aldık.

Kendine eş özdeğer problemleri ve polinom potansiyeline sahip parçacıkların Schrödinger denklemini tanıttıktan sonra, Lagrange interpolasyonu ve ortogonal polinomların bazı önemli özelliklerini hatırlattık. Herhangi bir dereceden bir ortogonal polinomun köklerinin bulunmasına yönelik, simetrik tridiagonal matris için özdeğer problemi kullanan bir yöntem sunduk. Hermite, Assosiye Laguerre, Chebyshev ve Legendre polinomlarının köklerinin bulunmasında kullanılan simetrik tridiagonal matrisleri oluşturduk.

Bundan sonra, yayınlanmış makaleleri çalışarak, Hermite ve Assosiye Laguerre polinomları kullanan sanki-spektral formülasyon oluşturduk. Ayrıca, bağımsız değişken üzerinden dönüşüm kullanarak sonsuz aralığı sonlu aralığa dönüştürdük ve Chebyshev ile Legendre polinomları kullanan sanki-spektral formülasyon elde ettik. Özel örnek olarak, yukarıda bahsedilen dört tür ortogonal polinomları kullanan sanki-spektral yöntemleri, polinom potansiyeline sahip kuvantum sistemlerin Schrödinger denklemini çözmek için uyguladık. Elde ettiğimiz sayısal sonuçları, başka yazarlar tarafından yayınlanan sayısal sonuçlarla karşılaştırdık ve kendi yöntemimizin yeterliliği ile ilgili yorumlarda bulunduk.

Anahtar Kelimeler: Schrödinger denklemi, ortogonal polinomlar, kendine eş özdeğer problemleri.

To my parents and my husband

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$\mathbb{N}$	:	the set of natural numbers
$\mathbb{N}_0$	:	the set of non-negative integers
$\mathbb{R}$	:	the set of real numbers
$\langle f, g \rangle$	:	inner product of the functions f and g
$C^n[a,b]$	:	the space of n times continuously differentiable functions on $[a,b]$
T_n	:	Chebyshev polynomial of degree n
L_n^ν	:	Associated Laguerre polynomial of degree n
P_n	:	Legendre polynomial of degree n
H_n	:	Hermite polynomial of degree n

CHAPTER 1

INTRODUCTION

1.1 Self-adjoint operators

It is well known that almost all problems in natural sciences and particularly in chemistry and physics are modeled by ordinary or partial differential equations which govern the behavior of certain physical quantities. In particular, every quantum mechanical system is modeled by the so-called Schrödinger equation which is an ordinary or partial differential equation. The eigenvalue problems for differential operators are also frequently encountered in various fields of science. For instance, the time independent Schrödinger equation is an eigenvalue problem for a differential operator of second order. In fact, many problems in physics and in particular in quantum mechanics are modeled by eigenvalue problems for self-adjoint operators.

Assume that a problem in any field is modeled by the eigenvalue problem

$$Ly = \lambda y, \quad By = 0, \tag{1.1}$$

where λ is a parameter, L is linear n-th order differential operator, $y \in C^n[a,b]$ that is, y is n- times continuously differentiable on $[a,b]$ and $By = 0$ represents the boundary conditions, if the problem is formulated on a finite closed interval $[a,b]$.

Definition 1.1.1 *For any $u, v \in L_2[a,b]$, the inner product $\langle u, v\rangle$ is defined as*

$$\langle u, v\rangle = \int_a^b u(x)\overline{v(x)}dx, \tag{1.2}$$

where $L_2[a,b]$ is the Hilbert space of all square integrable functions on $[a,b]$.

Definition 1.1.2 *[9] The linear differential operator L is called self-adjoint if, for all*

$u, v \in C^n[a, b]$ satisfying the boundary conditions $Bu = Bv = 0$, we have

$$\langle Lu, v \rangle = \langle u, Lv \rangle. \tag{1.3}$$

In this case the eigenvalue problem (1.1) is called self-adjoint eigenvalue problem. It is obvious that the problem (1.1) has the trivial solution $y \equiv 0$. If (1.1) has nontrivial solution for some constant λ then this constant λ is called an eigenvalue of the operator L and the nontrivial solution corresponding to λ is called an eigenfunction associated with λ.

Theorem 1.1.3 *[9] The eigenvalues of the self-adjoint problem* (1.1) *are all real and constitute at most countable set with no finite cluster points. In addition, eigenfunctions associated with distinct eigenvalues are orthogonal.*

Proof. Let λ_0 be an eigenvalue of (1.1) with corresponding eigenfunction y_0, That is,

$$Ly_0 = \lambda_0 y_0.$$

Since L is self-adjont, we have

$$\begin{aligned} \langle Ly_0, y_0 \rangle &= \langle y_0, Ly_0 \rangle, \\ \lambda_0 \langle y_0, y_0 \rangle &= \overline{\lambda_0} \langle y_0, y_0 \rangle. \end{aligned}$$

Hence,

$$(\lambda_0 - \overline{\lambda_0}) \langle y_0, y_0 \rangle = 0.$$

This implies $\lambda_0 = \overline{\lambda_0}$, that is, λ_0 is real. Now, let λ_1 and λ_2 be two distinct eigenvalues of (1.1) with corresponding eigenfunctions $y_1$and y_2. Then from self-adjointness condition we have

$$\langle Ly_1, y_2 \rangle = \langle y_1, Ly_2 \rangle,$$

or

$$\lambda_1 \langle y_1, y_2 \rangle = \lambda_2 \langle y_1, y_2 \rangle.$$

Hence,

$$(\lambda_1 - \lambda_2) \langle y_1, y_2 \rangle = 0.$$

Since $\lambda_1 \neq \lambda_2$, we deduce $\langle y_1, y_2 \rangle = 0$, which means that y_1 and y_2 are orthogonal. □

1.2 Schrödinger equation as a self-adjoint problem

The equation of motion in quantum mechanics is the so-called stationary Schrödinger equation and is an eigenvalue problem [2]. The probability densities and total energies of a quantum system are respectively the eigenfunctions and eigenvalues of this problem. However, the analytical solutions for this eigenvalue problem can be obtained only for very few cases. As a result, development of numerical methods to solve approximately this equation has been carried on by many researchers [3, 4, 10, 13, 24, 28, 32]. On the other hand, studies seeking analytical (polynomial) solutions of Schrödinger type differential equations are still being conducted.

The Schrödinger equation in one dimension for a particle moving in the presence of a potential $v(x)$ is known to be

$$H\psi(x) = \left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \tag{1.4}$$

where x is defined either on some finite interval or on the real line. It is known that on $L_2(\mathbb{R})$ the operator $-\dfrac{d^2}{dx^2}$ is self-adjoint. If $v(x)$ has no singularities on the domain under consideration, then the problem (1.4) with the condition that ψ is square integrable on $L_2(\mathbb{R})$, that is

$$\int_{\mathbb{R}} |\psi(x)|^2 dx < \infty,$$

is self-adjoint. In particular, for polynomial potentials, that is,

$$v(x) = \sum_{k=0}^{n} v_k x^k, \tag{1.5}$$

the eigenvalue problem (1.4) is self-adjoint and therefore, by the Theorem 1.1.3 has discrete real spectrum. Many studies in the literature deal with polynomial type potentials and especially with even-power polynomials. Even-power polynomial potentials are important because they are used in modeling charmonium systems [17, 19], and also in connection with anharmonic and double-well oscillators [2, 11, 16, 20, 26]. Actually, one of the few exactly solvable Schrödinger equations is the one of quantum harmonic oscillator where $v(x) = x^2$. Due to its importance, the Schrödinger equation with polynomial type potentials and the Schrödinger equation in general has been a subject of extensive studies including search for exact and approximate solutions [12, 14, 15, 16, 25, 26, 33, 34]. Various numerical methods such as perturbative, variational etc.[22, 33, 34] have been applied and results have been discussed. Some recent works deal with the use of pseudospectral methods for solving one-dimensional Schrödinger equation for polynomial potential [35, 36]. In this study, we apply the pseudospectral methods to even degree polynomial potentials and compare our numerical results with those reported in the literature. We consider both the previously discussed Hermite and Laguerre pseudospectral methods [35, 36] as well as Chebyshev and Legendre formulations which we develop in this work.

1.3 Quantum harmonic oscillator

One of the basic models in classical physics is the so-called harmonic oscillator. It is extremely useful in molecular physics because it is used to model the vibrational motion in a diatomic molecule. The quantum harmonic oscillator which is the quantum counter part of the classical one is among the simplest examples of quantum mechanical systems. It is one of the few exactly solvable problems in quantum mechanics. On the other hand, quantum harmonic oscillator is very important because many quantum systems with arbitrary potentials can be approximated by harmonic oscillators potential. The potential function of quantum harmonic oscillator is

$$v(x) = \frac{1}{2}mw^2x^2, \tag{1.6}$$

where m and w are physical constants. The time-independent Schrödinger equation for a one-dimensional quantum harmonic oscillator is known to be

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}mw^2x^2\psi(x) = E\psi(x), \quad x \in (-\infty, \infty), \tag{1.7}$$

where $\hbar$ is the so-called reduced Plank's constant. Using the transformation

$$x = \alpha\xi, \tag{1.8}$$

we have $\phi(\xi) = \psi(x)$ and hence,

$$\psi'(x) = \phi'(\xi)\frac{d\xi}{dx} = \frac{1}{\alpha}\phi'(\xi),$$

$$\psi''(x) = \frac{1}{\alpha}\phi''(\xi)\frac{d\xi}{dx} = \frac{1}{\alpha^2}\phi''(\xi).$$

Then the equation (1.7) takes form

$$-\frac{\hbar^2}{2m}\frac{1}{\alpha^2}\phi''(\xi) + \frac{1}{2}mw^2\alpha^2\xi^2\phi(\xi) = E\phi(\xi). \tag{1.9}$$

Multiplying by $-\frac{2m\alpha^2}{\hbar^2}$ we get

$$\phi''(\xi) - \frac{m^2w^2\alpha^4}{\hbar^2}\xi^2\phi(\xi) = -\frac{2m\alpha^2}{\hbar^2}E\phi(\xi). \tag{1.10}$$

Let $\alpha = \sqrt{\frac{\hbar}{mw}}$, then

$$\frac{m^2w^2\alpha^4}{\hbar^2} = \frac{m^2w^2}{\hbar^2}\frac{\hbar^2}{m^2w^2} = 1,$$

$$\frac{2m\alpha^2}{\hbar^2} = \frac{2m\hbar}{mw\hbar^2} = \frac{2}{\hbar w}.$$

Now, by taking $\varepsilon = -\frac{2}{\hbar w}E$, we transform the equation (1.10) to the form

$$\phi''(\xi) - \xi^2\phi(\xi) = \varepsilon\phi(\xi), \tag{1.11}$$

or,

$$\frac{\phi''(\xi)}{\phi(\xi)} - \xi^2 = \varepsilon. \tag{1.12}$$

We propose the following form for the solution $\phi(\xi)$,

$$\phi(\xi) = y(\xi)e^{-\frac{\xi^2}{2}}. \tag{1.13}$$

Then using logarithmic differentiation we compute

$$\ln\phi = \ln y - \frac{\xi^2}{2},$$

$$\frac{\phi'}{\phi} = \frac{y'}{y} - \xi,$$

$$\frac{\phi''\phi - (\phi')^2}{\phi^2} = \frac{y''y - (y')^2}{y^2} - 1,$$

where we dropped the ξ-dependence of the function for simplicity. Since $\frac{\phi'}{\phi} = \frac{y'}{y} - \xi$, then

$$\left(\frac{\phi'}{\phi}\right)^2 = \left(\frac{y'}{y}\right)^2 - 2\xi\frac{y'}{y} + \xi^2.$$

Hence, we have

$$\frac{\phi''}{\phi} = \left(\frac{y'}{y}\right)^2 - 2\xi\frac{y'}{y} + \xi^2 + \frac{y''}{y} - \left(\frac{y'}{y}\right)^2 - 1 = \frac{y''}{y} - 2\xi\frac{y'}{y} + \xi^2 - 1. \tag{1.14}$$

Substituting the expression (1.14) into the equation (1.12) we obtain

$$y''(\xi) - 2\xi y'(\xi) - (\varepsilon + 1)y(\xi) = 0,$$

or,

$$y''(\xi) - 2\xi y'(\xi) + (-\varepsilon - 1)y(\xi) = 0. \tag{1.15}$$

This equation is known as the Hermite differential equation whose solutions are Hermite polynomials $H_n(\xi)$ whenever $-\varepsilon - 1 = 2n$, $n \in \mathbb{N}_0$ and some of these polynomials are obtained as $H_0(\xi) = 1$, $H_1(\xi) = 2\xi$, $H_2(\xi) = 4\xi^2 - 2$, $H_3(\xi) = 8\xi^3 - 12\xi$. It is clear that for

$$\begin{aligned} n = 0 \quad \varepsilon_0 = -1 &\Longrightarrow E_0 = \frac{\hbar w}{2}, \\ n = 1 \quad \varepsilon_1 = -3 &\Longrightarrow E_1 = \frac{3}{2}\hbar w, \\ n = 2 \quad \varepsilon_2 = -5 &\Longrightarrow E_2 = \frac{5}{2}\hbar w, \end{aligned}$$

or, for any $n \in \mathbb{N}$, $\varepsilon_n = -(2n + 1)$ which implies $E_n = \frac{2n+1}{2}\hbar w$. Then, the energy eigenvalues of harmonic oscillator are

$$E_n = \frac{2n+1}{2}\hbar w, \tag{1.16}$$

and the corresponding eigenfunctions are

$$\phi_n(\xi) = H_n(\xi) e^{-\frac{\xi^2}{2}},$$

or in terms of the original variable x

$$\psi_n(x) = H_n\left(\frac{x}{\alpha}\right) e^{-\frac{x^2}{2\alpha^2}}. \tag{1.17}$$

1.4 Anharmonic oscillator

The quantum mechanical anharmonic oscillators in the one-dimensional case are represented by the potential

$$v(x) = v_2 x^2 + v_4 x^4 + \cdots + v_{2m} x^{2m}, m \geqslant 2. \tag{1.18}$$

This model has been attracting the interest of scientists for many years [12, 15, 16, 17, 21]. The reason for this is the analogy between anharmonic oscillators and one dimensional quantum field theories [3, 4]. On the other hand, various atomic and molecular problems in quantum chemistry also make use of anharmonic oscillators. Because of their wide range of applications, quantum anharmonic oscillators have been studied by means of different computational methods. Some of these methods are Rayleigh-Ritz variational approach [34], WKB methods [13, 22], Hill's determinant [11, 39], perturbative techniques [24], finite-difference methods [18]. Among other studies related with this model we can mention the work of Banerjee et.al. [3, 4] where a method using appropriately scaled basis for computation of each eigenvalue is derived. Also, a method proposed by Taşeli and Demiralp [31] and called Wronskian approach proved to be a powerful tool to solve anharmonic oscillator problem. In a recent work by Brandon and Saad [7] the problem of exact solvability of anharmonic oscillator with decatic (10th degree) polynomial potential has been discussed.

The Schrödinger equation for quantum systems with polynomial potentials is given as

$$\left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \quad x \in (-\infty, \infty), \tag{1.19}$$

where E is constant, ψ is square integrable function on $(-\infty, \infty)$ that is,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty, \tag{1.20}$$

and $v(x) = \sum_{n=1}^{p} v_{2n} x^{2n}$, is the potential function.

In our work we study the anharmonic oscillators with even power polynomial potentials. We construct the pseudospectral formulation for the equation (1.19) with four different types of orthogonal polynomials: Hermite, Associated Laguerre, Chebyshev and Legendre.

This thesis is organized as follows: In Chapter 2, we give some preliminary results on orthogonal polynomials and the idea behind the pseudospectral methods. We also develop a technique to compute the zeros of orthogonal polynomials and explain in details computation of zeros of Hermite, Associated Laguerre, Chebyshev and Legendre polynomials of any degree. In Chapter 3, we derive pseudospectral schemes with Hermite, Associated Laguerre, Chebyshev and Legendre polynomial for the problem (1.19). Chapter 4 is devoted to numerical results and discussion.

CHAPTER 2

PSEUDOSPECTRAL METHODS FOR SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS

The pseudospectral methods are used to find approximate solutions of ordinary and partial differential equations as well as integral equations. Although these methods were originally developed for the solution of partial differential equations [6], lately they have been proved to be important for solving ordinary differential equations arising from mathematical physics, integral equations and optimal control problems [27, 37, 38]. The idea behind the pseudospectral methods is the use of Lagrange polynomial interpolation for the dependent variable (unknown function) of the equation under consideration. The interpolating polynomial is constructed by using orthogonal polynomials.

2.1 Lagrange interpolation

First we recall the Lagrange interpolating polynomial.

Let f be a function whose values at a finite set of points $\{x_0, x_1, x_2, \ldots, x_n\}$ are given as $\{f(x_0), f(x_1), f(x_2), \ldots, f(x_n)\}$. The Lagrange interpolating polynomial is defined as [8].

$$L(x) = \sum_{i=0}^{n} \ell_i(x) f(x_i) = \ell_0(x) f(x_0) + \cdots + \ell_n(x) f(x_n), \tag{2.1}$$

where

$$\ell_i(x) = \frac{(x - x_0)\cdots(x - x_{i-1})(x - x_{i+1})\cdots(x - x_n)}{(x_i - x_0)\cdots(x_i - x_{i-1})(x_i - x_{i+1})\cdots(x_i - x_n)}, \tag{2.2}$$

for $i = 0, \ldots, n$. Here, the points $x_0, x_1 \ldots, x_n$ are called *interpolation points* or *nodes*.

The following theorem states that the Lagrange interpolating polynomial for a given set of interpolation points $x_0, x_1 \cdots, x_n$ is unique. The proof can be found in any numerical analysis book.

Theorem 2.1.1 *[8] If $x_0, x_1, \ldots, x_n$ are $n+1$ distinct nodes and f is a function whose values are given at these nodes, then a unique polynomial $L(x)$ of degree at most n exists with*

$$f(x_k) = L(x_k), \quad \textit{for each} \quad k = 0, 1, \ldots, n.$$

If the error in Lagrange interpolation is denoted by $E(x)$, then $f(x) \approx L(x)$ and $|f(x) - L(x)| < |E(x)|$ where,

$$E(x) = \frac{f^{n+1}(\xi)}{(n+1)!}(x - x_0) \cdots (x - x_n), \tag{2.3}$$

and ξ is any number in the interval containing $x_0, x_1, \ldots, x_n$.

In the next theorem, we prove the error formula for Lagrange interpolating polynomial.

Theorem 2.1.2 *[8] Let $x_0, x_1, \ldots, x_n$ be $n+1$ distinct nodes in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$. Then, for each x in $[a, b]$, a number $\xi(x)$ in (a, b) exists with*

$$f(x) = L(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)(x - x_1) \cdots (x - x_n), \tag{2.4}$$

where $L(x)$ is the interpolating polynomial given in (2.1).

Proof. Note first that if $x = x_k$, for any $k = 0, 1, \ldots, n$, then $f(x_k) = L(x_k)$, and choosing $\xi(x_k)$ arbitrarily in (a, b) yields (2.4). If $x \neq x_k$, for all $k = 0, 1. \ldots, n$, define the function g for t in $[a, b]$ by

$$\begin{aligned} g(t) &= f(t) - L(t) - [f(x) - L(x)] \frac{(t - x_0)(t - x_1) \cdots (t - x_n)}{(x - x_0)(x - x_1) \cdots (x - x_n)} \\ &= f(t) - L(t) - [f(x) - L(x)] \textstyle\prod_{i=0}^{n} \dfrac{(t - x_i)}{(x - x_i)}. \end{aligned}$$

Since $f \in C^{n+1}[a, b]$, and $L \in C^{\infty}$, it follows that $g \in C^{n+1}[a, b]$. For $t = x_k$ we have

$$g(x_k) = f(x_k) - L(x_k) - [f(x) - L(x)] \prod_{i=0}^{n} \frac{(x_k - x_i)}{(x - x_i)} = 0 - [f(x) - L(x)] .0 = 0.$$

Thus $g \in C^{n+1}[a,b]$, and g has $n+2$ zeros which are $x, x_0, x_1, \cdots, x_n$.

Hence, there exists a number ξ in (a,b) for which $g^{(n+1)}(\xi) = 0$. So that,

$$0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - L^{(n+1)}(\xi) - [f(x) - L(x)] \frac{d^{n+1}}{dt^{n+1}} \left[\prod_{i=0}^{n} \frac{(t - x_i)}{(x - x_i)} \right]_{t=\xi}. \tag{2.5}$$

However $L(x)$ is a polynomial of degree at most n, so the $(n+1)$st derivative, $L^{(n+1)}(x) \equiv 0$. Also, $\prod_{i=0}^{n}[(t - x_i)/(x - x_i)]$ is a polynomial of degree $(n+1)$, so

$$\prod_{i=0}^{n} \frac{(t - x_i)}{(x - x_i)} = \left[\frac{1}{\prod_{i=0}^{n}(x - x_i)} \right] t^{n+1} + (\text{lower-degree terms in} \quad t),$$

and

$$\frac{d^{n+1}}{dt^{n+1}} \prod_{i=0}^{n} \frac{(t - x_i)}{(x - x_i)} = \frac{(n+1)!}{\prod_{i=0}^{n}(x - x_i)}.$$

Equation (2.5) now becomes

$$0 = f^{(n+1)}(\xi) - 0 - [f(x) - L(x)] \frac{(n+1)!}{\prod_{i=0}^{n}(x - x_i)},$$

and, upon solving for $f(x)$, we have

$$f(x) = L(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n}(x - x_i).$$

□

In the description of pseudospectral methods, the terms $\ell_i(x)$ appearing in the Lagrange interpolating polynomials are taken as orthogonal polynomials.

2.2 Orthogonal polynomials

We first recall the definition of orthogonality. Define the inner product on $C[a,b]$ as

$$\langle f, g \rangle = \int_a^b f(x) g(x) w(x) dx \tag{2.6}$$

on a closed interval $[a,b]$ where $w(x) \geq 0$ on $[a,b]$ is the weight function.

If $\langle f, g \rangle = 0$ then f and g are orthogonal functions.

A set $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots\}$ is orthogonal set of polynomials if

$$\int_a^b P_i(x) P_j(x) w(x) dx = N_i \delta_{ij}, \quad \delta_{ij} = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}, \tag{2.7}$$

where N_i are positive constants.

Below we give some examples of orthogonal polynomials known as classical orthogonal polynomials [1].

(1) Legendre polynomials $P_n(x)$ are orthogonal with weight function $w(x) = 1$ on $[-1, 1]$. They satisfy orthogonality relation of the form

$$\int_{-1}^{1} P_i(x)P_j(x)dx = \frac{2}{2i+1}\delta_{ij}. \tag{2.8}$$

The first three Legendre polynomials are

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \frac{1}{2}(3x^2 - 1). \end{aligned}$$

(2) Associated Laguerre polynomials $L_n^\alpha(x)$ are orthogonal under weight function $w(x) = e^{-x}x^\alpha$ on $[0, \infty)$, where $\alpha > -1$ is a real number. They satisfy orthogonality relation of the form

$$\int_0^\infty L_i^\alpha(x)L_j^\alpha(x)e^{-x}x^\alpha dx = \frac{\Gamma(i+\alpha+1)}{i!}\delta_{ij}. \tag{2.9}$$

The first three Associated Laguerre polynomials with $\alpha = 0$ are

$$\begin{aligned} L_0(x) &= 1, \\ L_1(x) &= -x + 1, \\ L_2(x) &= \frac{1}{2}(x^2 - 4x + 2). \end{aligned}$$

(3) Hermite polynomials are orthogonal with weight function $w(x) = e^{-x^2}$ on $(-\infty, \infty)$. They satisfy orthogonality relation of the form

$$\int_{-\infty}^\infty H_i(x)H_j(x)e^{-x^2}dx = 2^i i!\sqrt{\pi}\delta_{ij}.$$

The first three Hermite polynomials are

$$\begin{aligned} H_0(x) &= 1, \\ H_1(x) &= 2x, \\ H_2(x) &= 4x^2 - 2. \end{aligned}$$

(4) Chebyshev polynomials are orthogonal with weight function $w(x) = \left(\sqrt{1-x^2}\right)^{-1}$ on $[-1,1]$. They satisfy orthogonality relation of the form

$$\int_{-1}^{1} \frac{T_i(x)T_j(x)dx}{\sqrt{1-x^2}} = \begin{cases} \frac{1}{2}\pi\delta_{ij} & \text{if} \quad i \neq 0 \\ \pi\delta_{ij} & \text{if} \quad i = 0 \end{cases}$$

The first three Chebyshev polynomials are

$$\begin{aligned} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_2(x) &= 2x^2 - 1. \end{aligned}$$

Theorem 2.2.1 *[1] If $P_n(x)$ is a member of a set of orthogonal polynomials on $[a,b]$ and x_i, $i = 1,2,\dots,n$ are zeros of $P_n(x)$, that is $P_n(x_i) = 0$, then all of these zeros are real, distinct and lie in $[a,b]$.*

Proof. Assume that $P_n(x)$ changes sign k times on $[a,b]$. Since $P_n(x)$ can have at most n distinct real zeros, we have $0 \leq k \leq n$. We will show that $k = n$. Define the polynomial

$$Q_k(x) = \begin{cases} 1 & \text{if} \quad k = 0 \\ \prod_{j=1}^{k}(x - x_j) & \text{if} \quad k \neq 0 \end{cases}, \tag{2.10}$$

where the points $x_j \in [a,b]$ are chosen as the points where $P_n(x)$ changes sign. It is then clear that $Q_k(x)P_n(x)$ is nonnegative on $[a,b]$. Since $w(x)Q_k(x)P_n(x) \geq 0$, we have

$$\int_a^b w(x)Q_k(x)P_n(x) > 0. \tag{2.11}$$

But from orthogonality, we know that $P_n(x)$ is orthogonal to all polynomials of degree smaller than n. Hence, we have $k = n$. Then, $P_n(x)$ has exactly n distinct real zeros in $[a,b]$. □

Assume that $\{P_0(x), P_1(x), \dots, P_n(x), \dots\}$ is a set of orthogonal polynomials. Then we have the following theorem about recurrence relation, the proof of which can be found in [23].

Theorem 2.2.2 *The following relation holds for any three consecutive orthogonal polynomials:*

$$xP_n(x) = \alpha_n P_{n+1}(x) + \beta_n P_n(x) + \gamma_n P_{n-1}(x), \quad n = 1, 2, \ldots, \tag{2.12}$$

where

$$\alpha_n = \frac{a_n}{a_{n+1}}, \quad \beta_n = \frac{b_n}{a_n} - \frac{b_{n+1}}{a_{n+1}}, \quad \gamma_n = \frac{\mathcal{N}_n^2}{\mathcal{N}_{n-1}^2}\frac{a_{n-1}}{a_n}, \tag{2.13}$$

and

$$P_n(x) = a_n x^n + b_n x^{n-1} + \cdots . \tag{2.14}$$

Now, we define

$$A_n(x, y) = (y - x)\sum_{k=0}^{n}\frac{1}{\mathcal{N}_k^2}P_k(x)P_k(y). \tag{2.15}$$

We will prove the following alternative representation for $A_n(x, y)$.

Proposition 2.2.3 *For every $n \in \mathbb{N}$, we have*

$$A_n(x, y) = \frac{a_n}{a_{n+1}}\frac{1}{\mathcal{N}_n^2}\left[P_n(x)P_{n+1}(y) - P_n(y)P_{n+1}(x)\right]. \tag{2.16}$$

Proof. We use the Mathematical Induction Principle. First, take $n = 1$. Then we have

$$\frac{A_1(x, y)}{y - x} = \sum_{k=0}^{1}\frac{1}{\mathcal{N}_k^2}P_k(x)P_k(y) = \frac{1}{\mathcal{N}_0^2}P_0(x)P_0(y) + \frac{1}{\mathcal{N}_1^2}P_1(x)P_1(y).$$

We will show that

$$A_1(x, y) = \frac{a_1}{a_2}\frac{1}{\mathcal{N}_1^2}\left[P_1(x)P_2(y) - P_2(x)P_1(y)\right]. \tag{2.17}$$

From the recurrence relation

$$xP_1(x) = \alpha_1 P_2(x) + \beta_1 P_1(x) + \gamma_1 P_0(x),$$

we have

$$\begin{aligned}
\alpha_1 P_2(y) &= \frac{a_1}{a_2}P_2(y) = (y - \beta_1)P_1(y) - \gamma_1 P_0(y)\\
\alpha_1 P_2(x) &= \frac{a_1}{a_2}P_2(x) = (x - \beta_1)P_1(x) - \gamma_1 P_0(x).
\end{aligned}$$

We use these expressions on the right-hand-side of (2.17):

$$\frac{1}{\mathcal{N}_1^2}[P_1(x)(y-\beta_1)P_1(y) - P_1(x)\gamma_1 P_0(y) - P_1(y)(x-\beta_1)P_1(x) + P_1(y)\gamma_1 P_0(x)]$$
$$= \frac{1}{\mathcal{N}_1^2}(y-x)P_1(x)P_1(y) - \frac{\gamma_1}{\mathcal{N}_1^2}[P_1(x)P_0(y) - P_1(y)P_0(x)]$$
$$= \frac{1}{\mathcal{N}_1^2}(y-x)P_1(x)P_1(y) - \frac{1}{\mathcal{N}_1^2}\frac{\mathcal{N}_1^2}{\mathcal{N}_0^2}\frac{a_0}{a_1}[P_1(x)P_0(y) - P_1(y)P_0(x)].$$

Notice that

$$P_1(x) = a_1 x + b_1, \quad P_0(x) = a_0.$$

Then,

$$P_1(x)P_0(y) - P_1(y)P_0(x) = a_0(a_1 x + b_1) - a_0(a_1 y + b_1) = a_0 a_1 (x-y).$$

In this case, we obtain

$$\frac{a_1}{a_2}\frac{1}{\mathcal{N}_1^2}\left[P_1(x)P_2(y) - P_2(x)P_1(y)\right]$$
$$= \frac{1}{\mathcal{N}_1^2}(y-x)P_1(x)P_1(y) - \frac{1}{\mathcal{N}_0^2}\frac{a_0}{a_1}a_0 a_1(x-y)$$
$$= \frac{1}{\mathcal{N}_1^2}(y-x)P_1(x)P_1(y) + \frac{1}{\mathcal{N}_0^2}(y-x)P_0(x)P_0(y)$$
$$= (y-x)\sum_{k=0}^{1}\frac{1}{\mathcal{N}_k^2}P_k(x)P_k(y)$$
$$= A_1(x,y).$$

Assume that the formula (2.16) holds for some $n = k$, that is,

$$A_k(x,y) = \frac{a_k}{a_{k+1}}\frac{1}{\mathcal{N}_k^2}\left[P_k(x)P_{k+1}(y) - P_k(y)P_{k+1}(x)\right], \tag{2.18}$$

for some $k \in \mathbb{N}$.

We will show that

$$A_{k+1}(x,y) = \frac{a_{k+1}}{a_{k+2}}\frac{1}{\mathcal{N}_{k+1}^2}\left[P_{k+1}(x)P_{k+2}(y) - P_{k+1}(y)P_{k+2}(x)\right]. \tag{2.19}$$

Using recurrence relation (2.12), we have

$$\alpha_{k+1}P_{k+2}(y) = \frac{a_{k+1}}{a_{k+2}}P_{k+2}(y) = (y-\beta_{k+1})P_{k+1}(y) - \gamma_{k+1}P_k(y)$$

$$\alpha_{k+1}P_{k+2}(x) = \frac{a_{k+1}}{a_{k+2}}P_{k+2}(x) = (x-\beta_{k+1})P_{k+1}(x) - \gamma_{k+1}P_k(x).$$

If we use these expressions on the right-hand-side of (2.19), then we get

$$\frac{a_{k+1}}{a_{k+2}}\frac{1}{\mathcal{N}_{k+1}^2}\left[P_{k+1}(x)P_{k+2}(y)-P_{k+1}(y)P_{k+2}(x)\right]$$

$$=\frac{1}{\mathcal{N}_{k+1}^2}\left[P_{k+1}(x)(y-\beta_{k+1})P_{k+1}(y)-\gamma_{k+1}P_{k+1}(x)P_k(y)\right.$$

$$\left.-P_{k+1}(y)(x-\beta_{k+1})P_{k+1}(x)+\gamma_{k+1}P_{k+1}(y)P_k(x)\right]$$

$$=\frac{1}{\mathcal{N}_{k+1}^2}\left[(y-x)P_{k+1}(x)P_{k+1}(y)\right]+\frac{1}{\mathcal{N}_{k+1}^2}\gamma_{k+1}\left[P_{k+1}(y)P_k(x)-P_{k+1}(x)P_k(y)\right]$$

$$=\frac{1}{\mathcal{N}_{k+1}^2}\left[(y-x)P_{k+1}(x)P_{k+1}(y)\right]+\frac{1}{\mathcal{N}_{k+1}^2}\frac{\mathcal{N}_{k+1}^2}{\mathcal{N}_k^2}\frac{a_k}{a_{k+1}}\left[P_{k+1}(y)P_k(x)-P_{k+1}(x)P_k(y)\right]$$

$$=\frac{1}{\mathcal{N}_{k+1}^2}\left[(y-x)P_{k+1}(x)P_{k+1}(y)\right]+\frac{1}{\mathcal{N}_k^2}\frac{a_k}{a_{k+1}}\left[P_{k+1}(y)P_k(x)-P_{k+1}(x)P_k(y)\right]$$

$$=\frac{1}{\mathcal{N}_{k+1}^2}\left[(y-x)P_{k+1}(x)P_{k+1}(y)\right]+A_k(x,y)$$

$$=(y-x)\frac{1}{\mathcal{N}_{k+1}^2}\left[P_{k+1}(x)P_{k+1}(y)\right]+(y-x)\sum_{m=0}^{k}\frac{1}{\mathcal{N}_m^2}\left[P_m(x)P_m(y)\right]$$

$$=(y-x)\sum_{m=0}^{k+1}\frac{1}{\mathcal{N}_m^2}\left[P_m(x)P_m(y)\right]$$
$$=A_{k+1}(x,y).$$

Hence, the proof is done. □

Theorem 2.2.4 *If $P_n(x)$ is a member of a set of orthogonal polynomials on $[a,b]$ then the zeros of $P_n(x)$ and $P_{n+1}(x)$ are interlaced, that is, $P_n(x)$ has a zero between two consecutive zeros of $P_{n+1}(x)$.*

Proof. From the Proposition 2.2.3 we know that

$$\frac{A_n(x,y)}{(y-x)}=\frac{\frac{\alpha_n}{\mathcal{N}_n^2}\left[P_n(x)P_{n+1}(y)-P_n(y)P_{n+1}(x)\right]}{y-x}. \tag{2.20}$$

If we take the limit of $\dfrac{A_n(x,y)}{(y-x)}$ as $y \to x$ and use the L'Hopitals rule we obtain

$$\begin{aligned}
\lim_{y\to x} \frac{A_n(x,y)}{(y-x)} &= \lim_{y\to x} \frac{\frac{\alpha_n}{\mathcal{N}_n^2}\left[P_n(x)P_{n+1}(y) - P_n(y)P_{n+1}(x)\right]}{y-x} \\
&= \lim_{y\to x} \frac{\frac{\alpha_n}{\mathcal{N}_n^2}\left[P_n(x)P'_{n+1}(y) - P'_n(y)P_{n+1}(x)\right]}{1} \\
&= \frac{\alpha_n}{\mathcal{N}_n^2}\left[P_n(x)P'_{n+1}(x) - P'_n(x)P_{n+1}(x)\right].
\end{aligned}$$

Also, taking limit as $y \to x$ of

$$\frac{A_n(x,y)}{(y-x)} = \sum_{k=0}^{n} \frac{1}{\mathcal{N}_k^2} P_k(x)P_k(y),$$

we obtain

$$\lim_{y\to x} \frac{A_n(x,y)}{(y-x)} = \sum_{k=0}^{n} \frac{1}{\mathcal{N}_k^2} P_k^2(x).$$

Therefore, we conclude

$$\sum_{k=0}^{n} \frac{P_k^2(x)}{\mathcal{N}_k^2} = \frac{\alpha_n}{\mathcal{N}_n^2}\left[P_n(x)P'_{n+1}(x) - P'_n(x)P_{n+1}(x)\right]. \tag{2.21}$$

If we put two consecutive zeros x_j and x_{j+1} of P_{n+1} in (2.21), then we get,

$$\begin{aligned}
\sum_{k=0}^{n} \frac{P_k^2(x_j)}{\mathcal{N}_k^2} &= \frac{\alpha_n}{\mathcal{N}_n^2} P_n(x_j)P'_{n+1}(x_j) \\
\sum_{k=0}^{n} \frac{P_k^2(x_{j+1})}{\mathcal{N}_k^2} &= \frac{\alpha_n}{\mathcal{N}_n^2} P_n(x_{j+1})P'_{n+1}(x_{j+1})
\end{aligned}$$

Therefore, the signs of $P_n(x_j)P'_{n+1}(x_j)$ and $P_n(x_{j+1})P'_{n+1}(x_{j+1})$ are the same (as the sign of $\alpha_n = \dfrac{a_{n+1}}{a_n}$). However, since x_j and x_{j+1} are two consecutive zeros of P_{n+1} then P'_{n+1} must have a zero at some x between x_j and x_{j+1}. Therefore, P'_{n+1} changes sign between x_j and x_{j+1} and so does $P_n(x)$. We conclude that P_n has a zero between any two consecutive zeros of P_{n+1}. □

2.3 Construction of pseudospectral formulation

Let the Lagrange interpolating polynomial for $y = f(x)$ be defined as

$$L(x) = \sum_{n=0}^{N} \ell_n(x) y_n, \quad y_n = f(x_n), \quad n = 0, \ldots, N, \tag{2.22}$$

where

$$\ell_n(x) = \frac{\prod_{m=0, m\neq n}^{N} (x - x_m)}{\prod_{m=0, m\neq n}^{N} (x_n - x_m)}. \tag{2.23}$$

It is clear that $\ell_n(x_n) = 1$.

For $x \neq x_n$, if we multiply and divide (2.23) by $(x - x_n)$, we obtain

$$\begin{aligned} \ell_n(x) &= \frac{(x - x_0)\cdots(x - x_n)\cdots(x - x_N)}{(x - x_n)(x_n - x_0)\cdots(x_n - x_{n-1})(x_n - x_{n+1})\cdots(x_n - x_N)} \\ &= \frac{F_{N+1}(x)}{(x - x_n)F'_{N+1}(x_n)}. \end{aligned}$$

Indeed, we can easily compute

$$\begin{aligned} F'_{N+1}(x) &= ((x - x_0)\cdots(x - x_N))' \\ &= \sum_{k=0}^{N}(x - x_0)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_N), \end{aligned}$$

and hence

$$F'_{N+1}(x_n) = (x_n - x_0)\cdots(x_n - x_{n-1})(x_n - x_{n+1})\cdots(x_n - x_N).$$

Then $L(x) = \sum_{n=0}^{N} \ell_n(x) y_n$, where

$$\ell_n(x) = \begin{cases} \dfrac{F_{N+1}(x)}{(x - x_n)F'_{N+1}(x_n)} & if \quad x \neq x_n \\ 1 & if \quad x = x_n \end{cases}. \tag{2.24}$$

Since, by the Theorem 2.2.1, any orthogonal polynomial of degree N has exactly N real and distinct zeros, then such a polynomial can be written as:

$$F_N(x) = a_N(x - x_0)(x - x_1)\cdots(x - x_{N-1}). \tag{2.25}$$

Therefore, if we take the function F_{N+1} in (2.24) as an orthogonal polynomial then the points $x_0, \ldots, x_N$ will be the real distinct zeros of this polynomial.

2.4 Computation of zeros of orthogonal polynomials

We now discuss the computation of zeros $x_0, x_1, \ldots, x_N$ of any orthogonal polynomial $F_{N+1}(x)$. We will employ the recurrence relation of orthogonal polynomials and derive a matrix eigenvalue problem to find these zeros.

To compute the zeros of any orthogonal polynomial F_{N+1} we use the recurrence relation given in (2.12).

$$\alpha_n F_{n+1}(x) + \beta_n F_n(x) + \gamma_n F_{n-1}(x) = xF_n(x).$$

Assuming that $F_{-1}(x) \equiv 0$, we write this relation for $n = 0, 1, \ldots, N$:

$$\begin{aligned} \beta_0 F_0(x) + \alpha_0 F_1(x) &= xF_0(x), \\ \gamma_1 F_0(x) + \beta_1 F_1(x) + \alpha_1 F_2(x) &= xF_1(x), \\ \vdots \quad & \quad \vdots \\ \gamma_N F_{N-1}(x) + \beta_N F_N(x) + \alpha_N F_{N+1}(x) &= xF_N(x). \end{aligned} \tag{2.26}$$

In matrix form, this system becomes

$$\begin{bmatrix} \beta_0 & \alpha_0 & 0 & 0 & \cdots & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \beta_2 & \alpha_2 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_N & \beta_N \end{bmatrix} \begin{bmatrix} F_0(x) \\ F_1(x) \\ F_2(x) \\ \vdots \\ F_N(x) \end{bmatrix} = x \begin{bmatrix} F_0(x) \\ F_1(x) \\ F_2(x) \\ \vdots \\ F_N(x) \end{bmatrix} - \alpha_N \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ F_{N+1}(x) \end{bmatrix}.$$

If we require that $F_{N+1}(x) = 0$, we obtain a matrix eigenvalue problem of the form

$$RF = xF, \tag{2.27}$$

where R is the tridiagonal matrix

$$R = \begin{bmatrix} \beta_0 & \alpha_0 & 0 & 0 & \cdots & 0 \\ \gamma_1 & \beta_1 & \alpha_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \beta_2 & \alpha_2 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_N & \beta_N \end{bmatrix},$$

and $F = [F_0(x) \cdots F_1(x) \quad \ldots F_N(x)]^T$. The matrix R is in general unsymmetric. However, it is possible to use a similarity transformation to transform the unsymmetric eigenvalue problem (2.27) into a symmetric one. Indeed, let

$$G = \text{diag}\{g_0, g_1, \ldots, g_N\}, \tag{2.28}$$

be a nonsingular diagonal matrix. Define

$$Y = G^{-1}F.$$

Then

$$RGY = RF = xF = xGY.$$

Hence,

$$G^{-1}RGY = xG^{-1}GY = xY,$$

or,

$$SY = xY,$$

where $S = G^{-1}RG$. Clearly the entries of S are computed as

$$s_{ij} = \frac{1}{g_i} r_{ij} g_j,$$

and moreover, S is also tridiagonal, that is,

$$s_{ij} = 0 \quad \text{if} \quad j > i + 1 \quad \text{and} \quad j < i - 1.$$

We require that S is symmetric, that is,

$$s_{i+1,i} = s_{i,i+1}, \quad i = 0, 1, \ldots, N - 1.$$

Then,

$$\frac{g_i}{g_{i+1}} r_{i+1,i} = \frac{g_{i+1}}{g_i} r_{i,i+1}, \quad i = 0, 1, \ldots, N - 1,$$

or,

$$g_i^2 \gamma_{i+1} = g_{i+1}^2 \alpha_i,$$

which gives

$$g_{i+1} = g_i \sqrt{\frac{\gamma_{i+1}}{\alpha_i}}, \quad i = 0, 1, \ldots, N - 1. \tag{2.29}$$

From this equation we compute the entries g_i of the diagonal matrix G recursively, starting with some arbitrary $g_0 \neq 0$. Since in our study we use Hermite, Laguerre, Chebyshev and Legendre polynomials, we derive symmetric eigenvalue problems for the computation of zeros of these polynomials. The derivation is presented in the following subsections.

2.4.1 Zeros of Hermite polynomials

Traditionally, Hermite polynomials are denoted by $H_n(x)$. The recurrence relation for Hermite polynomials is [1]

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x). \tag{2.30}$$

Rewriting this relation as

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

we see that $\alpha_n = \frac{1}{2}, \beta_n = 0$ and $\gamma_n = n$ for $n = 0, 1, \ldots, N$. Then the matrix R has the form

$$R = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 & \cdots & 0 \\ 1 & 0 & \frac{1}{2} & 0 & \cdots & 0 \\ 0 & 2 & 0 & \frac{1}{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \cdots & N & 0 \end{bmatrix}. \tag{2.31}$$

We compute the entries of the diagonal matrix G defined in (2.28) by using the recurrence formula (2.29) as

$$g_0 = \frac{1}{\sqrt{2}}, \quad g_1 = 1, \quad g_i = (\sqrt{2})^{i-1}\sqrt{i!}, \quad i = 2, \ldots, N.$$

Thus, to find the zeros of the Hermite polynomial H_{N+1} we will solve the symmetric eigenvalue problem

$$SY = xY,$$

where

$$S = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & \cdots & 0 \\ \frac{1}{\sqrt{2}} & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \sqrt{\frac{3}{2}} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \sqrt{\frac{N-1}{2}} & 0 & \sqrt{\frac{N}{2}} \\ 0 & \cdots & \cdots & 0 & \sqrt{\frac{N}{2}} & 0 \end{bmatrix}.$$

2.4.2 Zeros of Laguerre polynomials

For the zeros of the Associated Laguerre polynomials we use a similar procedure. The Associated Laguerre polynomials are denoted by $L_n^{(\alpha)}(x)$, where $\alpha > -1$. The recurrence relation for these orthogonal polynomials is [1]

$$(n+1)L_{n+1}^{(\alpha)}(x) = (\alpha + 2n + 1 - x)L_n^{(\alpha)}(x) - (\alpha + n)L_{n-1}^{(\alpha)}(x). \tag{2.32}$$

Rewrite this relation as

$$-(\alpha + n)L_{n-1}^{(\alpha)}(x) + (\alpha + 2n + 1)L_n^{(\alpha)}(x) - (n+1)L_{n+1}^{(\alpha)}(x) = xL_n^{(\alpha)}(x).$$

Then we have $\alpha_n = -(n+1), \beta_n = \alpha + 2n + 1$ and $\gamma_n = -(\alpha + n)$ for $n = 0, 1, \cdots, N$. The matrix R is of the form

$$R = \begin{bmatrix} (\alpha+1) & -1 & 0 & 0 & \cdots & 0 \\ -(\alpha+1) & (\alpha+3) & -2 & 0 & \cdots & 0 \\ 0 & -(\alpha+2) & (\alpha+5) & -3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & -(\alpha+N-1) & (\alpha+2N-1) & -N \\ 0 & 0 & 0 & \cdots & -(\alpha+N) & (\alpha+2N+1) \end{bmatrix}. \tag{2.33}$$

In order to have a symmetric eigenvalue problem, we compute the entries of the similarity transformation matrix G defined in (2.29) as

$$g_0 = \frac{1}{\sqrt{\alpha+1}}, \quad g_1 = 1, \ldots, \quad g_i = \sqrt{\frac{(\alpha+2)\cdots(\alpha+i)}{i!}}, \quad i = 2, \ldots, N.$$

Then, the symmetric matrix S is obtained as

$$S = \begin{bmatrix} \alpha+1 & -\sqrt{\alpha+1} & 0 & \cdots & \cdots & 0 \\ -\sqrt{\alpha+1} & \alpha+3 & -\sqrt{2(\alpha+2)} & 0 & \cdots & 0 \\ 0 & -\sqrt{2(\alpha+2)} & \alpha+5 & -\sqrt{3(\alpha+3)} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & -\sqrt{N(\alpha+N)} & \alpha+2N+1 \end{bmatrix}.$$

To find the zeros of the Laguerre polynomial L_{N+1}^{α} we will solve the symmetric eigenvalue problem

$$SY = xY.$$

2.4.3 Zeros of Chebyshev polynomials

We denote the Chebyshev polynomials by $T_n(x)$. The zeros of the Chebyshev polynomial T_{N+1} of degree $N + 1$ are known to be [1]

$$x_n = \cos\left(\frac{\pi(n + 1/2)}{N + 1}\right), \quad n = 0, 1, \ldots, N. \tag{2.34}$$

However, using the procedure described above, these zeros can also be obtained as matrix eigenvalues. The recurrence relation for Chebyshev polynomials is

$$\frac{1}{2}T_{n-1}(x) + \frac{1}{2}T_{n+1}(x) = xT_n, \quad n = 1, 2, \ldots$$

and

$$T_1 = xT_0,$$

so that we have $\alpha_0 = 1, \beta_0 = 0$, $\alpha_n = \frac{1}{2}, \beta_n = 0$ and $\gamma_n = \frac{1}{2}$ for $n = 1, \ldots, N$. Then the matrix R in (2.27) is almost symmetric and has the form

$$R = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & 0 & \cdots & 0 \\ 0 & 1/2 & 0 & 1/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1/2 \\ 0 & 0 & 0 & \cdots & 1/2 & 0 \end{bmatrix}. \tag{2.35}$$

To find the zeros of T_{N+1} we solve the matrix eigenvalue problem

$$RT = xT.$$

2.4.4 Zeros of Legendre polynomials

Legendre polynomials are usually denoted by $P_n(x)$. The recurrence relation for Legendre polynomials is [1]

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x). \tag{2.36}$$

Again, we rewrite this equation in the form

$$\frac{n}{2n + 1}P_{n-1}(x) + \frac{n + 1}{2n + 1}P_{n+1}(x) = xP_n(x),$$

and we have $\alpha_n = \dfrac{n+1}{2n+1}, \beta_n = 0$ and $\gamma_n = \dfrac{n}{2n+1}$ for $n = 0, 1, \ldots, N$.

Then the matrix R becomes

$$R = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & 0 & \cdots & 0 \\ 0 & \frac{2}{5} & 0 & \frac{3}{5} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{N+1}{2N+1} \\ 0 & 0 & 0 & \cdots & \frac{N}{2N+1} & 0 \end{bmatrix}. \tag{2.37}$$

The entries of the diagonal matrix G are now obtained from (2.29) as

$$g_i = \frac{1}{\sqrt{2i+1}}, \quad i = 0, \ldots, N.$$

Thus, the zeros of the Legendre polynomial P_{N+1} are obtained as the eigenvalues of the symmetric matrix

$$S = \begin{bmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & \cdots & \cdots & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{15}} & 0 & \cdots & 0 \\ 0 & \frac{2}{\sqrt{15}} & 0 & \frac{3}{\sqrt{35}} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \frac{N-1}{\sqrt{(2N-3)(2N-1)}} & 0 & \frac{N}{\sqrt{(2N-1)(2N+1)}} \\ 0 & \cdots & \cdots & 0 & \frac{N}{\sqrt{(2N-1)(2N+1)}} & 0 \end{bmatrix}.$$

2.5 Computation of derivatives

As we are going to apply the pseudospectral methods to ordinary differential equations, we need to replace the dependent variable $y(x)$ by the Lagrange interpolating polynomial. If we consider second order differential equations, the derivatives up to second order of the function $y(x)$ are involved.

Let $y(x) = \sum_{n=0}^{N} y_n \ell_n(x)$, where

$$\ell_n(x) = \begin{cases} \dfrac{F_{N+1}(x)}{(x-x_n)F'_{N+1}(x_n)} & if \quad x \neq x_n \\ 1 & if \quad x = x_n \end{cases}.$$

Clearly, $y'(x) = \sum_{n=0}^{N} y_n \ell_n'(x)$ and $y''(x) = \sum_{n=0}^{N} y_n \ell_n''(x)$. Therefore, we need to compute the derivatives $\ell_n'(x)$ and $\ell_n''(x)$.

For $x \neq x_n$ we have

$$\ell_n'(x) = \frac{F_{N+1}'(x)(x - x_n) - F_{N+1}(x)}{(x - x_n)^2 F_{N+1}'(x_n)} = \frac{1}{F_{N+1}'(x_n)} \left[\frac{F_{N+1}'(x)}{x - x_n} - \frac{F_{N+1}(x)}{(x - x_n)^2} \right].$$

For $x = x_n$ we use the L'Hopitals rule and obtain

$$\begin{aligned}
\ell_n'(x_n) &= \lim_{x \to x_n} \frac{\ell_n(x) - \ell_n(x_n)}{x - x_n} \\
&= \lim_{x \to x_n} \frac{\dfrac{F_{N+1}(x)}{(x - x_n)F_{N+1}'(x_n)} - 1}{x - x_n} \\
&= \lim_{x \to x_n} \frac{F_{N+1}(x) - (x - x_n)F_{N+1}'(x_n)}{(x - x_n)^2 F_{N+1}'(x_n)} \\
&= \lim_{x \to x_n} \frac{F_{N+1}'(x) - F_{N+1}'(x_n)}{2(x - x_n)F_{N+1}'(x_n)} \\
&= \lim_{x \to x_n} \frac{F_{N+1}''(x)}{2F_{N+1}'(x_n)} \\
&= \frac{F_{N+1}''(x_n)}{2F_{N+1}'(x_n)}.
\end{aligned}$$

Hence, we get

$$\ell_n'(x) = \begin{cases} \dfrac{F_{N+1}'(x)(x - x_n) - F_{N+1}(x)}{(x - x_n)^2 F_{N+1}'(x_n)} & if \quad x \neq x_n \\[2ex] \dfrac{F_{N+1}''(x_n)}{2F_{N+1}'(x_n)} & if \quad x = x_n \end{cases}.$$

For the second order derivatives, whenever $x \neq x_n$ we compute

$$\begin{aligned}
\ell_n''(x) &= \frac{d}{dx}\left[\frac{F'_{N+1}(x)}{(x-x_n)F'_{N+1}(x_n)} - \frac{F_{N+1}(x)}{(x-x_n)^2F'_{N+1}(x_n)}\right] \\
&= \frac{F''_{N+1}(x)(x-x_n) - F'_{N+1}(x)}{(x-x_n)^2F'_{N+1}(x_n)} - \frac{F'_{N+1}(x)(x-x_n)^2 - F_{N+1}(x)2(x-x_n)}{(x-x_n)^4F'_{N+1}(x_n)} \\
&= \left[\frac{F''_{N+1}(x)}{(x-x_n)} - \frac{2F'_{N+1}(x)}{(x-x_n)^2} + \frac{2F_{N+1}(x)}{(x-x_n)^3}\right]\frac{1}{F'_{N+1}(x_n)}.
\end{aligned}$$

For $x = x_n$, we use L'Hopitals rule which gives

$$\begin{aligned}
\ell_n''(x_n) &= \lim_{x\to x_n}\frac{\ell_n'(x)-\ell_n'(x_n)}{(x-x_n)} \\
&= \lim_{x\to x_n}\frac{\frac{1}{F'_{N+1}(x_n)}\left[\frac{F'_{N+1}(x)}{(x-x_n)} - \frac{F_{N+1}(x)}{(x-x_n)^2}\right] - \frac{1}{2}\frac{F''_{N+1}(x_n)}{F'_{N+1}(x_n)}}{(x-x_n)} \\
&= \lim_{x\to x_n}\frac{1}{2F'_{N+1}(x_n)}\left[\frac{2(x-x_n)F'_{N+1}(x) - 2F_{N+1}(x) - (x-x_n)^2F''_{N+1}(x_n)}{(x-x_n)^3}\right] \\
&= \lim_{x\to x_n}\frac{1}{2F'_{N+1}(x_n)}\left[\frac{2F'_{N+1}(x) + 2(x-x_n)F''_{N+1}(x) - 2F'_{N+1}(x) - 2(x-x_n)F''_{N+1}(x_n)}{3(x-x_n)^2}\right] \\
&= \lim_{x\to x_n}\frac{1}{2F'_{N+1}(x_n)}\left[\frac{2F''_{N+1}(x) + 2(x-x_n)F'''_{N+1}(x) - 2F''_{N+1}(x_n)}{6(x-x_n)}\right] \\
&= \lim_{x\to x_n}\frac{1}{2F'_{N+1}(x_n)}\left[\frac{2F'''_{N+1}(x) + 2F'''_{N+1}(x) + 2(x-x_n)F^{(4)}_{N+1}(x)}{6}\right] \\
&= \frac{1}{3}\frac{F'''_{N+1}(x_n)}{F'_{N+1}(x_n)}.
\end{aligned}$$

Hence, we obtain

$$\ell_n''(x) = \begin{cases} \left[\frac{F''_{N+1}(x)}{(x-x_n)} - \frac{2F'_{N+1}(x)}{(x-x_n)^2} + \frac{2F_{N+1}(x)}{(x-x_n)^3}\right]\frac{1}{F'_{N+1}(x_n)} & \text{if} \quad x \neq x_n \\ \frac{1}{3}\frac{F'''_{N+1}(x_n)}{F'_{N+1}(x_n)} & \text{if} \quad x = x_n \end{cases}.$$

From the fact that x_m, $m = 0, 1, \ldots, N$ are zeros of F_{N+1}, we easily see that

$$\ell_n(x_m) = \delta_{mn} = \begin{cases} 0 & \text{if} \quad m \neq n \\ 1 & \text{if} \quad m = n \end{cases}, \tag{2.38}$$

$$\ell_n'(x_m) = \begin{cases} \dfrac{1}{(x_m - x_n)} \dfrac{F_{N+1}'(x_m)}{F_{N+1}'(x_n)} & if \quad m \neq n \\ \\ \dfrac{1}{2} \dfrac{F_{N+1}''(x_n)}{F_{N+1}'(x_n)} & if \quad m = n \end{cases}, \tag{2.39}$$

$$\ell_n''(x_m) = \begin{cases} \dfrac{F_{N+1}''(x_m)}{(x_m - x_n)F_{N+1}'(x_n)} - \dfrac{2F_{N+1}'(x_m)}{(x_m - x_n)^2 F_{N+1}'(x_n)} & if \quad m \neq n \\ \\ \dfrac{1}{3} \dfrac{F_{N+1}'''(x_n)}{F_{N+1}'(x_n)} & if \quad m = n \end{cases}. \tag{2.40}$$

CHAPTER 3

DERIVATION OF PSEUDOSPECTRAL SCHEMES WITH DIFFERENT ORTHOGONAL POLYNOMIALS

3.1 Hermite pseudospectral formulation

In this section we will derive the pseudospectral formulation of the problem (1.19) in which we will use Hermite polynomials. We follow the computations by Taşeli and H. Alıcı [35]. We consider again the eigenvalue problem

$$[-\frac{d^2}{dx^2} + v(x)]\psi(x) = E\psi(x), \qquad x \in (-\infty, \infty), \tag{3.1}$$

where E is a constant and $v(x)$ is the potential function. As we did with harmonic oscillator equation, we make a substitution

$$\psi(x) = e^{-\frac{x^2}{2}} y(x).$$

Using logarithmic differentiation in

$$\ln \psi = -\frac{x^2}{2} + \ln y,$$

and employing the formulas (1.14) obtained in Section 1.3, we get:

$$-y'' + 2xy' + [(v(x) - x^2 - (E + 1)]y = 0, \tag{3.2}$$

or

$$-y'' + 2xy' + (v(x) - x^2)y = \varepsilon y, \tag{3.3}$$

where $\varepsilon = E + 1$. Now, we suppose that

$$y(x) = \sum_{n=0}^{N} y_n \ell_n(x), \tag{3.4}$$

where

$$\ell_n(x) = \frac{H_{N+1}(x)}{(x - x_n)H'_{N+1}(x_n)}.$$

In this representation $H_{N+1}(x)$ is the Hermite polynomial of degree $N + 1$ and x_n, $n = 0, 1, \ldots, N$ are the zeros of $H_{N+1}(x)$. Then we have

$$y' = \sum_{n=0}^{N} y_n \ell_n'(x),$$

and

$$y'' = \sum_{n=0}^{N} y_n \ell_n''(x).$$

If we substitute (3.4) and its derivatives into equation (3.3), we obtain

$$-\sum_{n=0}^{N} y_n \ell_n''(x) + 2x \sum_{n=0}^{N} y_n \ell_n'(x) + (v(x) - x^2) \sum_{n=0}^{N} y_n \ell_n(x) = \varepsilon \sum_{n=0}^{N} y_n \ell_n(x),$$

or

$$\sum_{n=0}^{N} y_n [-\ell_n''(x) + 2x\ell_n'(x) + (v(x) - x^2)\ell_n(x)] = \varepsilon \sum_{n=0}^{N} y_n \ell_n(x).$$

We write this equation at the zeros $x = x_m$ for $m = 0, \ldots, N$, which gives

$$\sum_{n=0}^{N} y_n [-\ell_n''(x_m) + 2x_m \ell_n'(x_m) + (v(x_m) - x_m^2)\ell_n(x_m)] = \varepsilon \sum_{n=0}^{N} y_n \ell_n(x_m). \tag{3.5}$$

This system can be written in matrix form as

$$KY = \varepsilon Y,$$

where the entries of $(N+1)\times(N+1)$ matrix K will be computed by using the derivative representations obtained in (2.38), (2.39) and (2.40). The $(N + 1) \times 1$ vector Y contains the constants $y_0, y_1, \ldots, y_N$.

For $m \neq n$ we calculate the entries of the matrix K as follows:

$$\begin{aligned} K_{mn} &= -\frac{H''_{N+1}(x_m)}{(x_m - x_n)H'_{N+1}(x_n)} + 2\frac{H'_{N+1}(x_m)}{(x_m - x_n)^2 H'_{N+1}(x_n)} + 2x_m \frac{H'_{N+1}(x_m)}{(x_m - x_n)H'_{N+1}(x_n)} \\ &= -\frac{1}{(x_m - x_n)H'_{N+1}(x_n)} [H''_{N+1}(x_m) - 2x_m H'_{N+1}(x_m)] + \frac{2}{(x_m - x_n)^2} \frac{H'_{N+1}(x_m)}{H'_{N+1}(x_n)}. \end{aligned}$$

From the differential equation of Hermite polynomials we have

$$H''_{N+1}(x_m) - 2x_m H'_{N+1}(x_m) = -2(N + 1)H_{N+1}(x_m) = 0,$$

because x_m's are the zeros of H_{N+1}. Then, for $m \neq n$ we conclude

$$K_{mn} = \frac{2}{(x_m - x_n)^2} \frac{H'_{N+1}(x_m)}{H'_{N+1}(x_n)}. \tag{3.6}$$

Now, we use (2.38), (2.39) and (2.40) to compute the diagonal entries K_{nn} of the matrix K.

$$K_{nn} = -\frac{H'''_{N+1}(x_n)}{3H'_{N+1}(x_n)} + \frac{2x_n H''_{N+1}(x_n)}{2H'_{N+1}(x_n)} + (v(x_n) - x_n^2).$$

Regarding the differential equation of Hermite polynomials, we express the third derivative in terms of lower derivatives and after some calculations we obtain

$$\begin{aligned} K_{nn} &= \frac{1}{3H'_{N+1}(x_n)}[x_n H''_{N+1}(x_n) + 2NH'_{N+1}(x_n)] + (v(x_n) - x_n^2) \\ &= \frac{1}{3H'_{N+1}(x_n)}[2x_n^2 H'_{N+1}(x_n) + 2NH'_{N+1}(x_n)] + (v(x_n) - x_n^2) \\ &= \frac{2}{3}(x_n^2 + N) + (v(x_n) - x_n^2) \end{aligned} \tag{3.7}$$

As a result, from (3.6) and (3.7) we have the matrix K as

$$K_{mn} = \begin{cases} \dfrac{2}{(x_m - x_n)^2} \dfrac{H'_{N+1}(x_m)}{H'_{N+1}(x_n)} & if \quad m \neq n \\ \dfrac{2}{3}(x_n^2 + N) + (v(x_n) - x_n^2) & if \quad m = n \end{cases}.$$

To simplify further the entries of K, we use a similarity transformation

$$L = \text{diag}\{H'_{N+1}(x_1), H'_{N+1}(x_2), \cdots\}$$

which helps to get rid of $\dfrac{H'_{N+1}(x_m)}{H'_{N+1}(x_n)}$ in the off-diagonal entries of K. Then taking $Y = LZ$, the eigenvalue problem $KY = \varepsilon Y$ becomes

$$KLZ = \varepsilon LZ,$$

and thus,

$$PZ = \varepsilon Z,$$

where $P = L^{-1}KL$. Then the entries of P are easily computed as follows.

$$P_{mn} = \begin{cases} \dfrac{2}{(x_m - x_n)^2} & if \quad m \neq n \\ \dfrac{2}{3}(x_n^2 + N) + (v(x_n) - x_n^2) & if \quad m = n \end{cases}.$$

Therefore, the problem of finding the eigenvalues of the Schrödinger equation is transformed to a matrix eigenvalue problem.

Recall that the zeros x_m, $m = 0, 1, \ldots, N$ of the Hermite polynomial H_{N+1} have been computed in Section 2.4.1 as eigenvalues of a symmetric tridiagonal matrix.

3.2 Laguerre Pseudospectral formulation

In this section, we will derive a pseudospectral method by using Associated Laguerre polynomials. Consider again the Schrödinger equation for quantum polynomial potential

$$\left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \quad x \in (-\infty, \infty), \tag{3.8}$$

where $v(x)$ is an even polynomial of x. We follow the computations in [36].

Since $v(-x) = v(x)$, let $t = (cx)^2$, where $c > 0$, $t \in (0, \infty)$. Let $\phi(t) = \psi(x)$ and $u(t) = v(x)$. Then, by the Chain Rule, we compute

$$\frac{d\psi}{dx} = \frac{d\phi}{dt}\frac{dt}{dx} = 2c^2x\frac{d\phi}{dt},$$

$$\begin{aligned}\frac{d^2\psi}{dx^2} &= \frac{d^2\phi}{dt^2}\left(\frac{dt}{dx}\right)^2 + \frac{d\phi}{dt}\frac{d^2t}{dx^2} \\ &= (2c^2x)^2\frac{d^2\phi}{dt^2} + 2c^2\frac{d\phi}{dt}.\end{aligned}$$

Substituting these expressions into the equation (3.8), we obtain

$$-(2c^2x)^2\frac{d^2\phi}{dt^2} - 2c^2\frac{d\phi}{dt} + u(t)\phi(t) = E\phi(t), \quad t \in (0, \infty),$$

and after some simplification we conclude

$$t\phi'' + \frac{1}{2}\phi' - \frac{1}{4c^2}u(t)\phi = \varepsilon\phi, \tag{3.9}$$

where

$$\varepsilon = -\frac{E}{4c^2}.$$

We next assume that $\phi(t)$ is in the form $\phi(t) = t^\alpha e^{-t/2}y(t)$, for some $\alpha > -1$. To compute $\phi'(t), \phi''(t)$ we use logarithmic differentiation as described below,

$$\ln\phi(t) = \ln(t^\alpha e^{-t/2}y(t)) = \alpha\ln t - \frac{t}{2} + \ln y(t)$$

$$\frac{\phi'(t)}{\phi(t)} = \frac{\alpha}{t} - \frac{1}{2} + \frac{y'(t)}{y(t)}$$

$$\frac{\phi(t)\phi''(t) - (\phi'(t))^2}{(\phi(t))^2} = \frac{-\alpha}{t^2} + \frac{y(t)y''(t) - (y'(t))^2}{(y(t))^2},$$

which results in

$$
\begin{aligned}
\frac{\phi''(t)}{\phi(t)} &= -\frac{\alpha}{t^2} + \frac{y''(t)}{y(t)} - \left(\frac{y'(t)}{y(t)}\right)^2 \\
&\quad + \left\{\left(\frac{\alpha}{t} - \frac{1}{2}\right)^2 + 2\left(\frac{\alpha}{t} - \frac{1}{2}\right)\frac{y'(t)}{y(t)} + \left(\frac{y'(t)}{y(t)}\right)^2\right\} \\
&= -\frac{\alpha}{t^2} + \frac{y''(t)}{y(t)} + \frac{\alpha^2}{t^2} - \frac{\alpha}{t} + \frac{1}{4} + \left(\frac{2\alpha}{t} - 1\right)\frac{y'(t)}{y(t)} \\
&= \frac{-\alpha + \alpha^2}{t^2} - \frac{\alpha}{t} + \frac{1}{4} + \frac{y''(t)}{y(t)} + \left(\frac{2\alpha}{t} - 1\right)\frac{y'(t)}{y(t)}.
\end{aligned}
\tag{3.10}
$$

We use these derivatives to rewrite the equation (3.9) as

$$
t\left\{\frac{-\alpha + \alpha^2}{t^2} - \frac{\alpha}{t} + \frac{1}{4} + \frac{y''(t)}{y(t)} + \left(\frac{2\alpha}{t} - 1\right)\frac{y'(t)}{y(t)}\right\} + \frac{1}{2}\left\{\frac{\alpha}{t} - \frac{1}{2} + \frac{y'(t)}{y(t)}\right\} - \frac{1}{4c^2}u = \varepsilon,
$$

which simplifies as

$$
t\frac{y''(t)}{y(t)} + \left(2\alpha - t + \frac{1}{2}\right)\frac{y'(t)}{y(t)} + \frac{2\alpha^2 - \alpha}{2t} + \frac{1}{4}t - (\alpha + \frac{1}{4}) - \frac{1}{4c^2}u = \varepsilon. \tag{3.11}
$$

In order to remove the singularity at $t = 0$, we choose α so that the term $\frac{2\alpha^2 - \alpha}{2t}$ vanishes. That is, we take $\alpha = 0$ or $\alpha = \frac{1}{2}$. For $\alpha = 0$ the equation (3.11) has the form

$$
ty''(t) + \left(-t + \frac{1}{2}\right)y'(t) + \left(\frac{1}{4}(t - 1) - \frac{1}{4c^2}u(t)\right)y(t) = \varepsilon y(t), \tag{3.12}
$$

and for $\alpha = \frac{1}{2}$ it becomes

$$
ty''(t) + \left(-t + \frac{3}{2}\right)y'(t) + \left(\frac{1}{4}(t - 3) - \frac{u(t)}{4c^2}\right) = \varepsilon y(t). \tag{3.13}
$$

Actually, we can represent the equations (3.12) and (3.13) as a single differential equation as

$$
ty'' + (-t + \nu + 1)\,y' + \left(\frac{1}{4}t - \frac{1}{4c^2}u(t) - \frac{\nu + 1}{2}\right)y(t) = \varepsilon y(t), \tag{3.14}
$$

where $\nu = -\frac{1}{2}$ or $\nu = \frac{1}{2}$, respectively.

The differential equation

$$
ty'' + (-t + \nu + 1)y' + ny = 0, \tag{3.15}
$$

is known as the Associated Laguerre differential equation whose solutions are the Associated Laguerre polynomials $L_n^{\nu}(t)$. Since the transformed equation (3.14) has differential operator of the same type as that in the Associated Laguerre differential equation, we will propose a solution $y(t)$ in the form

$$y(t) = \sum_{n=0}^{N} y_n \ell_n(t), \tag{3.16}$$

where

$$\ell_n(t) = \frac{L_{N+1}^{\nu}(t)}{(t - t_n)(L_{N+1}^{\nu})'(t_n)} \tag{3.17}$$

with $\nu = -\frac{1}{2}$ or $\nu = \frac{1}{2}$.

As stated in [36], the solutions of (3.14) for $\nu = -\frac{1}{2}$ or $\nu = \frac{1}{2}$ give the even and odd eigenfunctions, respectively, of (3.8) via the back substitution to the variable x. Therefore, to obtain the complete set of eigenvalues, we need to consider both cases for ν.

If we substitute (3.16) into (3.14), we obtain

$$\sum_{n=0}^{N} t y_n \ell_n''(t) + (\nu + 1 - t) \sum_{n=0}^{N} y_n \ell_n'(t) + \left[\frac{1}{4}t - \frac{1}{4c^2}u(t) - \frac{\nu + 1}{2}\right] \sum_{n=0}^{N} y_n \ell_n(t) = \varepsilon \sum_{n=0}^{N} y_n \ell_n(t),$$

or

$$\sum_{n=0}^{N} y_n [t\ell_n''(t) + (\nu + 1 - t)\ell_n'(t) + w(t)\ell_n(t)] = \varepsilon \sum_{n=0}^{N} y_n \ell_n(t),$$

where $w(t) = \frac{1}{4}t - \frac{1}{4c^2}u(t) - \frac{\nu + 1}{2}$. If we write this equation at the zeros $t = t_m$ for $m = 0, \ldots, N$, we get

$$\sum_{n=0}^{N} y_n [t_m \ell_n''(t_m) + (\nu + 1 - t_m)\ell_n'(t_m) + w(t_m)\ell_n(t_m)] = \varepsilon \sum_{n=0}^{N} y_n \ell_n(t_m). \tag{3.18}$$

This system can be written in matrix form as

$$KY = \varepsilon Y,$$

where the entries of $(N+1)\times(N+1)$ matrix K will be computed by using the derivative representations obtained in (2.38),(2.39) and (2.40).

For $m \neq n$ we calculate the entries of the matrix K as follows.

$$\begin{aligned} K_{mn} &= \frac{t_m (L_{N+1}^{\nu})''(t_m)}{(t_m - t_n)(L_{N+1}^{\nu})'(t_n)} - \frac{2t_m (L_{N+1}^{\nu})'(t_m)}{(t_m - t_n)^2 (L_{N+1}^{\nu})'(t_n)} + \frac{(\nu + 1 - t_m)(L_{N+1}^{\nu})'(t_m)}{(t_m - t_n)(L_{N+1}^{\nu})'(t_n)} \\ &= \frac{t_m (L_{N+1}^{\nu})''(t_m) + (\nu + 1 - t_m)(L_{N+1}^{\nu})'(t_m)}{(t_m - t_n)(L_{N+1}^{\nu})'(t_n)} - 2\frac{t_m (L_{N+1}^{\nu})'(t_m)}{(t_m - t_n)^2 (L_{N+1}^{\nu})'(t_n)}. \end{aligned}$$

From the differential equation of Associated Laguerre polynomials we have

$$t_m(L^{\nu}_{N+1})''(t_m) + (\nu + 1 - t_m)(L^{\nu}_{N+1})'(t_m) = -(N+1)(L^{\nu}_{N+1})(t_m) = 0,$$

because t_m is a the zeros of L_{N+1}. Then, for $m \neq n$, we conclude

$$K_{mn} = -\frac{2t_m}{(t_m - t_n)^2} \frac{(L^{\nu}_{N+1})'(t_m)}{(L^{\nu}_{N+1})'(t_n)}. \tag{3.19}$$

To compute the diagonal entries K_{nn} we recall the expressions (2.38), (2.39) and (2.40). We have

$$K_{nn} = \frac{t_n}{3} \frac{(L^{\nu}_{N+1})'''(t_n)}{(L^{\nu}_{N+1})'(t_n)} + \frac{\nu + 1 - t_n}{2} \frac{(L^{\nu}_{N+1})''(t_n)}{(L^{\nu}_{N+1})'(t_n)} + w(t_n).$$

From the differential equation (3.15) of Associated Laguerre polynomials, we obtain

$$t_n(L^{\nu}_{N+1})'''(t_n) = -(\nu + 2 - t_n)(L^{\nu}_{N+1})''(t_n) - N(L^{\nu}_{N+1})'(t_n).$$

Then

$$\begin{aligned} K_{nn} &= \frac{1}{(L^{\nu}_{N+1})'(t_n)} \left[-\frac{1}{3}(\nu + 2 - t_n) + \frac{1}{2}(\nu + 1 - t_n) \right] (L^{\nu}_{N+1})''(t_n) - \frac{N}{3} + w(t_n) \\ &= \frac{1}{(L^{\nu}_{N+1})'(t_n)} \frac{1}{6}(\nu - 1 - t_n) \frac{-(\nu + 1 - t_n)(L^{\nu}_{N+1})'(t_n)}{t_n} - \frac{N}{3} + w(t_n). \end{aligned}$$

We conclude

$$K_{nn} = -\frac{1}{6t_n}(\nu - 1 - t_n)(\nu + 1 - t_n) - \frac{N}{3} + w(t_n). \tag{3.20}$$

Clearly, the matrix K is not symmetric. We rewrite the off-diagonal entries of K by multiplying and dividing by $\sqrt{t_n}$ as

$$K_{mn} = -\frac{2t_m(L^{\nu}_{N+1})'(t_m)}{(t_m - t_n)^2(L^{\nu}_{N+1})'(t_n)} = -\frac{2\sqrt{t_m t_n}}{(t_m - t_n)^2} \frac{\sqrt{t_m}(L^{\nu}_{N+1})'(t_m)}{\sqrt{t_n}(L^{\nu}_{N+1)})'(t_n)}. \tag{3.21}$$

As a result, from (3.20) and (3.21) we have the entries of the matrix K as

$$K_{mn} = \begin{cases} -\dfrac{2\sqrt{t_m t_n}}{(t_m - t_n)^2} \dfrac{\sqrt{t_m}(L^{\nu}_{N+1})'(t_m)}{\sqrt{t_n}(L^{\nu}_{N+1})'(t_n)} & if \quad m \neq n \\ \\ -\dfrac{1}{6t_n}(\nu - 1 - t_n)(\nu + 1 - t_n) - \dfrac{N}{3} + w(t_n) & if \quad m = n \end{cases}.$$

In order to simplify further, we use the similarity transformation

$$L = \text{diag}\left\{ \sqrt{t_0}(L^{\nu}_{N+1})'(t_0),\ \sqrt{t_1}(L^{\nu}_{N+1})'(t_1), \ldots,\ \sqrt{t_N}(L^{\nu}_{N+1})'(t_N) \right\},$$

and define $Y = LZ$. This transforms the eigenvalue problem

$$KY = \varepsilon Y$$

into

$$KLZ = \varepsilon LZ,$$

and hence, we deduce the eigenvalue problem $PZ = \varepsilon Z$, where $P = L^{-1}KL$ is a symmetric matrix with entries

$$P_{mn} = \begin{cases} -\dfrac{2\sqrt{t_m t_n}}{(t_m - t_n)^2} & if \quad m \neq n \\ \\ -\dfrac{1}{6t_n}(\nu - 1 - t_n)(\nu + 1 - t_n) - \dfrac{N}{3} + w(t_n) & if \quad m = n \end{cases}.$$

In our computations, we use both cases in which $\nu = \dfrac{1}{2}$ and $\nu = -\dfrac{1}{2}$ leading to different types of Associated Laguerre polynomials. Computation of zeros $t_m, \quad m = 0, 1, \ldots, N$ requires finding the eigenvalues of the symmetric tridiagonal matrix S as explained in Section 2.4.2.

3.3 Chebyshev pseudospectral formulation

The Schrödinger equation for particles with polynomial potentials is defined on the whole real line. However, both Chebyshev and Legendre polynomials are orthogonal on the finite interval $[-1, 1]$. Therefore, we need a variable transformation to transform the infinite interval $(-\infty, \infty)$ to the finite interval $[-1, 1]$.

Consider the Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \quad x \in (-\infty, \infty). \tag{3.22}$$

In order to transform this equation into an equation of Chebyshev type on the finite interval $[-1, 1]$, we propose the following substitution on the independent variable.

$$t = \sin \alpha x, \quad t \in [-1, 1]. \tag{3.23}$$

where α is an optimization parameter which is useful for numerical purposes. We explain the role of this parameter in the next chapter. Then, if we denote

$$y(t) = \psi(x) \text{ and } u(t) = v(x),$$

we compute

$$\begin{aligned}\frac{d\psi(x)}{dx} &= \frac{dy}{dt}\frac{dt}{dx} = -\alpha\cos(\alpha x)\frac{dy}{dt}\\ \frac{d^2\psi(x)}{dx^2} &= \frac{d^2y}{dt^2}\left(\frac{dt}{dx}\right)^2 + \frac{dy}{dt}\frac{d^2t}{dx^2} = \alpha^2\cos^2(\alpha x)\frac{d^2y}{dt^2} - \alpha^2\sin(\alpha x)\frac{dy}{dt}.\end{aligned}$$

Then, the equation (3.22) becomes

$$\alpha^2\left[(1-t^2)\frac{d^2y}{dt^2} - t\frac{dy}{dt}\right] - u(t)y(t) = -Ey(t), \quad t \in [-1,1],$$

or,

$$(1-t^2)\frac{d^2y}{dt^2} - t\frac{dy}{dt} - \frac{u(t)}{\alpha^2}y(t) = \varepsilon y(t), \tag{3.24}$$

where $\varepsilon = -\dfrac{E}{\alpha^2}$.

Recalling the differential equations of Chebyshev polynomials

$$(1-t^2)T_n''(t) - tT_n'(t) + n^2T_n(t) = 0, \tag{3.25}$$

we notice the similarity of the differential operators in both equations (3.24) and (3.25) above.

Then, we propose $y(t) = \sum_{n=0}^{N} y_n\ell_n(t)$, where $\ell_n(t) = \dfrac{T_{N+1}(t)}{(t-t_n)T'_{N+1}(t_n)}$, and t_n, $n = 0,1,\ldots,N$ are the zeros of the Chebyshev polynomial $T_{N+1}(t)$ and are known to be

$$t_n = \cos\left(\frac{\pi(n+1/2)}{N+1}\right), \quad n = 0,1,\ldots,N. \tag{3.26}$$

Then we put this form of $y(t)$ into the equation (3.24) and evaluate at the points t_m for $m = 0,\ldots,N$ which gives

$$\sum_{n=0}^{N} y_n\left[(1-t_m^2)\ell_n''(t_m) - t_m\ell_n'(t_m) - \frac{u(t_m)}{\alpha^2}\delta_{mn}\right] = \varepsilon\sum_{n=0}^{N} y_n\delta_{mn}.$$

Therefore, we obtain a matrix eigenvalue problem in the form

$$KY = \varepsilon Y, \tag{3.27}$$

where $K_{mn} = (1-t_m^2)\ell_n''(t_m) - t_m\ell_n'(t_m) - \dfrac{u(t_m)}{\alpha^2}\delta_{mn}$. Using the derivatives of $\ell_n(t_m)$ which we have derived in (2.38), (2.39) and (2.40), we compute the entries of the matrix K as follows.

For $m \neq n$

$$K_{mn} = (1-t_m^2)\left[\frac{1}{(t_m-t_n)}\frac{T''_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{2}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}\right] - \frac{t_m}{(t_m-t_n)}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}$$

$$= \frac{(1-t_m^2)}{(t_m-t_n)}\frac{T''_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{t_m}{(t_m-t_n)}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}$$

$$= \frac{1}{T'_{N+1}(t_n)}\frac{1}{(t_m-t_n)}\left[(1-t_m^2)T''_{N+1}(t_m) - t_m T'_{N+1}(t_m)\right] - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}$$

$$= \frac{1}{T'_{N+1}(t_n)}\frac{1}{(t_m-t_n)}\left[-(N+1)^2 T_{N+1}(t_m)\right] - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}$$

$$= -\frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}.$$

For $m = n$

$$K_{nn} = \frac{(1-t_n^2)}{3}\frac{T'''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{u(t_n)}{\alpha^2}$$

$$= t_n\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{u(t_n)}{\alpha^2}$$

$$= \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2}$$

$$= \frac{t_n}{2}\frac{\frac{t_n}{1-t_n^2}T'_{N+1}(t_n) - \frac{(N+1)^2}{(1-t_n^2)}T_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2}$$

$$= \frac{t_n^2}{2(1-t_n^2)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2}.$$

Thus, we have

$$K_{mn} = \begin{cases} -\dfrac{2(1-t_m^2)}{(t_m-t_n)^2}\dfrac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} & \text{if} \quad m \neq n \\ \dfrac{t_n^2}{2(1-t_n^2)} - \dfrac{N(N+2)}{3} - \dfrac{u(t_n)}{\alpha^2} & \text{if} \quad m = n \end{cases}.$$

Since K is not a symmetric matrix, we apply the following procedure to obtain a symmetric matrix. We rewrite K_{mn} for $m \neq n$ as

$$K_{mn} = -\frac{2\sqrt{(1-t_m^2)(1-t_n^2)}}{(t_m - t_n)^2}\frac{\sqrt{(1-t_m^2)}T'_{N+1}(t_m)}{\sqrt{(1-t_n^2)}T'_{N+1}(t_n)}.$$

Then using a diagonal matrix

$$L = \text{diag}\left\{\sqrt{1-t_0^2}T'_{N+1}(t_0),\ \sqrt{1-t_1^2}T'_{N+1}(t_1), \cdots,\ \sqrt{1-t_N^2}T'_{N+1}(t_N)\right\},$$

and defining $Y = LZ$, we transform the problem

$$KY = \varepsilon Y,$$

into

$$PZ = \varepsilon Z,$$

where $P = L^{-1}KL$ is a symmetric matrix with entries

$$P_{mn} = \begin{cases} -\dfrac{2\sqrt{(1-t_m^2)(1-t_n^2)}}{(t_m - t_n)^2} & \text{if} \quad m \neq n \\ \dfrac{t_n^2}{2(1-t_n^2)} - \dfrac{N(N+2)}{3} - \dfrac{u(t_n)}{\alpha^2} & \text{if} \quad m = n \end{cases}.$$

Here the function $u(t)$ is in the form

$$u(t) = v(x) = v(\frac{1}{\alpha}\arcsin t).$$

3.4 Legendre pseudospectral formulation

In this section, we consider the Legendre basis set for the pseudospectral method to solve the Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \quad x \in (-\infty, \infty). \tag{3.28}$$

Since Legendre polynomials form an orthogonal set in $[-1, 1]$ and are solutions of the differential equation

$$(1-t^2)P''_n - 2tP'_n + n(n+1)P_n = 0, \tag{3.29}$$

we need to apply a transformation on the independent variable x, which transforms the differential operator of the (3.28) to Legendre type and the infinite interval $(-\infty, \infty)$ into $[-1, 1]$.

Let

$$t = \tanh(\alpha x),$$

where $\alpha > 0$ is an optimization parameter. Then $t \in (-1, 1)$ for $x \in (-\infty, \infty)$ and

$$x = \frac{1}{\alpha} \tanh^{-1} t = \frac{1}{2\alpha} \ln\left(\frac{1+t}{1-t}\right).$$

If we define $y(t) = \psi(x)$, $u(t) = v(x)$, then

$$\begin{aligned}
\frac{d\psi}{dx} &= \frac{dy}{dt}\frac{dt}{dx} = \alpha \text{sech}^2(\alpha x)\frac{dy}{dt} \\
\frac{d^2\psi}{dx^2} &= \left(\frac{dt}{dx}\right)^2 \frac{d^2y}{dt^2} + \frac{d^2t}{dx^2}\frac{dy}{dt} \\
&= \alpha^2 \text{sech}^4(\alpha x)\frac{d^2y}{dt^2} - 2\alpha^2 \text{sech}^2(\alpha x)\tanh(\alpha x)\frac{dy}{dt} \\
&= \alpha^2 \text{sech}^2(\alpha x)\left[(1-\tanh^2(\alpha x))\frac{d^2y}{dt^2} - 2\tanh(\alpha x)\frac{dy}{dt}\right] \\
&= \alpha^2(1-t^2)[(1-t^2)\frac{d^2y}{dt^2} - 2t\frac{dy}{dt}].
\end{aligned}$$

Using the new variables, we transform (3.28) into

$$(1-t^2)\left[(1-t^2)y''(t) - 2ty'(t)\right] - \frac{u(t)}{\alpha^2}y(t) = \varepsilon y(t), \tag{3.30}$$

where $\varepsilon = -\frac{E}{\alpha^2}$. The differential operator of the transformed equation resembles the differential operator of Legendre equation. Therefore, we propose

$$y(t) = \sum_{n=0}^{N} y_n \ell_n(t), \tag{3.31}$$

where

$$\ell_n(t) = \frac{P_{N+1}(t)}{(t-t_n)P'_{N+1}(t_n)},$$

$P_{N+1}(t)$ is the Legendre polynomial of degree $N+1$ and t_n, $n = 0, 1, \ldots, N$ are the zeros of $P_{N+1}(t)$. We put the sum (3.31) into the equation (3.30) and require its satisfaction at the nodes $t_0, t_1, \cdots, t_N$. This results in

$$\sum_{n=0}^{N} y_n \left\{(1-t_m^2)\left[(1-t_m^2)\ell_n''(t_m) - 2t_m\ell_n'(t_m)\right] - \frac{u(t_m)}{\alpha^2}\ell_n(t_m)\right\} = \varepsilon \sum_{n=0}^{N} y_n\ell_n(t_m), \quad m = 0, 1, \cdots, N.$$

As a result, we obtain an eigenvalue problem of the form

$$KY = \varepsilon Y,$$

where the $(N+1)\times(N+1)$ matrix K has entries

$$K_{mn} = (1-t_m^2)\left[(1-t_m^2)\ell_n''(t_m) - 2t_m\ell_n'(t_m)\right] - \frac{u(t_m)}{\alpha^2}\ell_n(t_m).$$

To compute the entries of K, we employ (2.38), (2.39) and (2.40).

For $m \neq n$

$$\begin{aligned}
K_{mn} &= (1-t_m^2)\left\{(1-t_m^2)\left[\frac{1}{t_m-t_n}\frac{P''_{N+1}(t_m)}{P'_{N+1}(t_n)} - \frac{2}{(t_m-t_n)^2}\frac{P'_{N+1}(t_m)}{P'_{N+1}(t_n)}\right] - \frac{2t_m}{(t_m-t_n)}\frac{P'_{N+1}(t_m)}{P'_{N+1}(t_n)}\right\} \\
&= (1-t_m^2)\left\{\frac{1}{(t_m-t_n)P'_{N+1}(t_n)}\left[(1-t_m^2)P''_{N+1}(t_m) - 2t_m P'_{N+1}(t_m)\right] - \frac{2(1-t_m^2)P'_{N+1}(t_m)}{(t_m-t_n)^2 P'_{N+1}(t_n)}\right\} \\
&= \frac{(1-t_m^2)}{(t_m-t_n)P'_{N+1}(t_n)}\left[-(N+1)(N+2)P_{N+1}(t_m)\right] - \frac{2(1-t_m^2)^2 P'_{N+1}(t_m)}{(t_m-t_n)^2 P'_{N+1}(t_n)} \\
&= -\frac{2(1-t_m^2)^2 P'_{N+1}(t_m)}{(t_m-t_n)^2 P'_{N+1}(t_n)}.
\end{aligned}$$

For $m = n$

$$\begin{aligned}
K_{nn} &= (1-t_n^2)\left[\frac{1-t_n^2}{3}\frac{P'''_{N+1}(t_n)}{P'_{N+1}(t_n)} - t_n\frac{P''_{N+1}(t_n)}{P'_{N+1}(t_n)}\right] - \frac{u(t_n)}{\alpha^2} \\
&= (1-t_n^2)\left[\frac{4t_n}{3}\frac{P''_{N+1}(t_n)}{P'_{N+1}(t_n)} - \frac{(N+1)(N+2)-2}{3} - t_n\frac{P''_{N+1}(t_n)}{P'_{N+1}(t_n)}\right] - \frac{u(t_n)}{\alpha^2} \\
&= (1-t_n^2)\left[\frac{t_n}{3}\frac{2t_n}{(1-t_n^2)} - \frac{(N+1)(N+2)-2}{3}\right] - \frac{u(t_n)}{\alpha^2} \\
&= \frac{2}{3}t_n^2 - \frac{(1-t_n^2)}{3}(N^2-3N) - \frac{u(t_n)}{\alpha^2}.
\end{aligned}$$

As we did in the previous section, we multiply and divide the off diagonal entries of K_{mn} by $(1-t_n^2)$ in order to make the matrix K symmetric.

Hence, we deduce

$$K_{mn} = \begin{cases} -\dfrac{2(1-t_m^2)(1-t_n^2)}{(t_m-t_n)^2}\dfrac{(1-t_m^2)P'_{N+1}(t_m)}{(1-t_n^2)P'_{N+1}(t_n)} & if \quad m \neq n \\[2ex] \dfrac{2}{3}t_n^2 - \dfrac{(1-t_n^2)}{3}(N^2-3N) - \dfrac{u(t_n)}{\alpha^2} & if \quad m = n \end{cases},$$

where $u(t_n) = v(x_n)$ and $x_n = \dfrac{1}{2\alpha}\ln\left(\dfrac{1+t_n}{1-t_n}\right)$. Again, in order to deal with a matrix of simple structure, we transform the eigenvalue problem

$$KY = \varepsilon Y,$$

into the problem

$$PZ = \varepsilon Z,$$

where $P = L^{-1}KL$, $Z = L^{-1}Y$ and

$$L = \text{diag}\left\{(1-t_0^2)P'_{N+1}(t_0), (1-t_1^2)P'_{N+1}(t_1), \cdots, (1-t_N^2)P'_{N+1}(t_N)\right\},$$

so that the matrix P has entries

$$P_{mn} = \begin{cases} -\dfrac{2(1-t_m^2)(1-t_n^2)}{(t_m-t_n)^2} & if \quad m \neq n \\ \\ \dfrac{2}{3}t_n^2 - \dfrac{(1-t_n^2)}{3}(N^2-3N) - \dfrac{u(t_n)}{\alpha^2} & if \quad m = n \end{cases}.$$

In this chapter, we obtained pseudospectral formulations with 4 different types of orthogonal polynomials for the same problem. It should be noticed that, in all cases we deduce a symmetric eigenvalue problem

$$PZ = \varepsilon Z,$$

where P contains the potential function $v(x)$ in its diagonal entries. Although we considered $v(x)$ to be an even degree polynomial, one can take the potential as any function on $(-\infty, \infty)$ without singularities.

CHAPTER 4

NUMERICAL RESULTS

In this chapter, we present the numerical results obtained by applying the four pseudospectral schemes discussed in the previous chapter. We consider the polynomial potential

$$v(x) = x^2 + v_4x^4 + v_6x^6 + v_8x^8, \tag{4.1}$$

where v_4, v_6 and v_8 are positive constants. The values of v_4, v_6, v_8 are chosen in 3 sets:

$$0 < v_i < 1, \quad v_i = 1 \quad \text{and} \quad v_i > 1 \quad \text{for} \quad i = 4, 6, 8. \tag{4.2}$$

In this way, we can observe the effects of small and large perturbations on the harmonic oscillator. In all tables, i shows the index of the eigenvalue, N the degree of the Lagrange interpolating polynomial. All calculations are done with MATLAB program and the related MATLAB files are given in the Appendix.

4.1 Eigenvalues of Schrödinger equation via Hermite pseudospectral method

Using Hermite pseudospectral formulation we computed the eigenvalues tabulated below. In Table 4.1, we considered the case $v_6 = v_8 = 0$ and four values for v_4 : $0.1, 0.5, 1, 5$. We observed that as the value of v_4 increases, we need larger degree N of interpolating polynomial H_N. The same holds for the other cases of parameters v_i in the potential $v(x)$. Table 4.2 shows the results for $v_4 = v_8 = 0$ and four different values of v_6. Similarly, in Table 4.3 we tabulated the eigenvalues of the potential $v(x) = x^2 + v_8x^8$. Finally, in Table 4.4 we give the eigenvalues of the potential $v(x) = x^2 + v_4x^4 + v_6x^6$ for two sets of the parameters v_4 and v_6.

Table 4.1: Eigenvalues for the potential $v(x) = x^2 + v_4 x^4$ with Hermite pseudospectral method

		$v_4 = 0.1$		$v_4 = 0.5$		$v_4 = 1$		$v_4 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.06528551	15	1.24185192	20	1.39235312	25	2.01837730
2		3.30687202		4.05188376		4.64881973		7.01307645
3		5.74795853		7.39687032		8.65479731		13.45909320
4		8.35266983		11.11885368		13.15466818		20.78985571
5		11.09865978		15.14726888		18.06200423		29.20174801
1	25	1.06528551	25	1.24185406	30	1.39235165	35	2.01833982
2		3.30687201		4.05193227		4.64881285		7.01349181
3		5.74795927		7.39690045		8.65505068		13.46807428
4		8.35267783		11.11516004		13.15679328		20.81471332
5		11.09859562		15.13690128		18.05742404		28.85976412

Table 4.2: Eigenvalues for the potential $v(x) = x^2 + v_6 x^6$ with Hermite pseudospectral method

		$v_6 = 0.1$		$v_6 = 0.5$		$v_6 = 1$		$v_6 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.10911312	15	1.30020487	20	1.43586820	25	1.91023404
2		3.59627548		4.45607185		5.03364869		6.94011965
3		6.64481508		8.65842972		9.95100079		14.07885458
4		10.22949776		13.84618394		15.85332177		22.98489000
5		14.23401464		20.33480400		22.55479546		34.44841043
1	25	1.10908716	25	1.30096972	30	1.43564880	35	1.91276328
2		3.59603630		4.46344091		5.03367987		6.96336437
3		6.64437193		8.68469795		9.96821797		14.18003443
4		10.23768356		13.80155128		15.99379401		23.04370562
5		14.30611359		19.67784975		22.89545417		33.01059877

Table 4.3: Eigenvalues for the potential $v(x) = x^2 + v_8 x^8$ with Hermite pseudospectral method

		$v_8 = 0.1$		$v_8 = 0.5$		$v_8 = 1$		$v_8 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.16957654	15	1.35997913	20	1.49485785	25	1.87317073
2		3.94703821		4.77510698		5.38493178		6.92118319
3		7.68823271		9.52420735		10.97520499		14.41584395
4		12.44533383		15.51006625		17.77862702		24.18822883
5		17.96719472		23.25208655		25.05905242		37.18768419
1	25	1.16900468	25	1.36795141	30	1.49119533	35	1.89065515
2		3.94016015		4.83882281		5.37183136		7.02984538
3		7.64315281		9.76297223		11.01461166		14.74110874
4		12.29573841		15.96421645		18.29386579		24.59300359
5		17.80727064		23.13072587		27.01871881		35.72589754

Table 4.4: Eigenvalues for the potential $v(x) = x^2 + v_4 x^4 + v_6 x^6$ with Hermite pseudospectral method

		$v_4 = 0.5, v_6 = 0.5$		$v_4 = 1, v_6 = 1$
i	N	E_i	N	E_i
1	15	1.42106160	15	1.61701738
2		4.88530039		5.66711812
3		9.43041159		11.05170867
4		14.83021651		17.00902965
5		21.63850875		23.76816088
1	25	1.42133242	25	1.61493730
2		4.89157673		5.65721173
3		9.48129007		11.11436399
4		14.95600331		17.66023792
5		21.15764505		24.98887221

4.2 Eigenvalues of Schrödinger equation via Laguerre pseudospectral method

In this section we present the numerical results obtained by using Laguerre pseudospectral formulation derived in Section 3.2.We considered again the same potential

$$v(x) = x^2 + v_4 x^4 + v_6 x^6 + v_8 x^8,$$

with the same values for the parameters v_4, v_6, v_8 as in the previous section. Recall that using the substitution $t = (cx)^2$, as discussed in Section 3.2 resulted in splitting the eigenvalues of the problem into two sets corresponding to even and odd eigenfunctions. Therefore, in order to obtain the complete set of eigenvalues, we performed numerical computations with $\nu = \frac{1}{2}$ and $\nu = -\frac{1}{2}$. The positive constant $c$is taken as $c = 1$. The results are obtained with MATLAB and tabulated in Tables 4.5-4.8. For comparison purposes, we used the same values for the coefficients v_4, v_6 and v_8 as in the previous section.

Table 4.5: Eigenvalues for the potential $v(x) = x^2 + v_4 x^4$ with Laguerre pseudospectral method

		$v_4 = 0.1$		$v_4 = 0.5$		$v_4 = 1$		$v_4 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.06528551	15	1.24185406	20	1.39235164	25	2.01834067
2		3.30687201		4.05193233		4.64881270		7.01347896
3		5.74795927		7.39690062		8.65504997		13.46773141
4		8.35267783		11.11515406		13.15680384		20.81398712
5		11.09859562		15.13684911		18.05755726		28.87475781
1	25	1.06528551	25	1.24185406	30	1.39235164	35	2.01834065
2		3.30687201		4.05193233		4.64881270		7.01347918
3		5.74795927		7.39690064		8.65504996		13.46773043
4		8.35267783		11.11515428		13.15680390		20.81396696
5		11.09859562		15.13684575		18.05755744		28.87499529

Table 4.6: Eigenvalues for the potential $v(x) = x^2 + v_6 x^6$ with Laguerre pseudospectral method

		$v_6 = 0.1$		$v_6 = 0.5$		$v_6 = 1$		$v_6 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.10908708	15	1.30098643	20	1.43562192	25	1.91246493
2		3.59603719		4.46371555		5.03340347		6.96086581
3		6.64438861		8.68606261		9.96656252		14.16861824
4		10.23788991		13.80949837		15.98895640		23.04601132
5		14.30690178		19.67071181		22.91344369		33.24453115
1	25	1.10908708	25	1.30098696	30	1.43562462	35	1.91245485
2		3.59603692		4.46368299		5.03339576		6.96085056
3		6.64439171		8.68639468		9.96662340		14.16913161
4		10.23787374		13.80828136		15.98943017		23.04155096
5		14.30703992		19.67792286		22.91023711		33.27203775

Table 4.7: Eigenvalues for the potential $v(x) = x^2 + v_8 x^8$ with Laguerre pseudospectral method

		$v_8 = 0.1$		$v_8 = 0.5$		$v_8 = 1$		$v_8 = 5$
i	N	E_i	N	E_i	N	E_i	N	E_i
1	15	1.16896883	15	1.36805427	20	1.49085291	25	1.88767856
2		3.93957221		4.83778247		5.36991059		7.01093882
3		7.64055200		9.78346789		10.98697652		14.67538660
4		12.27679199		16.07936530		18.20597357		24.58028327
5		17.77843622		23.44180815		26.68201616		36.08043091
1	25	1.16897037	25	1.36771617	30	1.49100746	35	1.88755248
2		3.93972374		4.83921985		5.36885449		7.01050971
3		7.63993455		9.77698096		10.99329709		14.68100653
4		12.28124256		16.07293923		18.19207670		24.54000270
5		17.76083613		23.53337302		26.73943454		36.29275834

Table 4.8: Eigenvalues for the potential $v(x) = x^2 + v_4x^4 + v_6x^6$ with Laguerre pseudospectral method

		$v_4 = 0.5, v_6 = 0.5$		$v_4 = 1, v_6 = 1$
i	N	E_i	N	E_i
1	15	1.42132476	15	1.61487778
2		4.89154195		5.65636156
3		9.48226881		11.10815098
4		14.96699519		17.62894186
5		21.18686753		25.10613806
1	25	1.42132029	25	1.61489423
2		4.89155939		5.65643520
3		9.48218802		11.10736845
4		14.96584081		17.63773604
5		21.19830062		25.06865123

4.3 Eigenvalues of Schrödinger equation via Chebyshev pseudospectral method

As we stated in Section 3.3, to our knowledge, the Chebyshev pseudospectral formulation for the Schrödinger equation with polynomial potential has not been used by other authors before. The substitution transforming the infinite interval $(-\infty, \infty)$ to $[-1, 1]$ employed in our study is $t = \sin(\alpha x)$, where $\alpha > 0$ is an optimization parameter. The effect of α is observed in the numerical results presented below. First, we noticed that by taking $0 < \alpha < 1$ the accuracy of the method increases when we take same number N. We tried various values for α in order to determine an optimum one. We observed that the optimal value for α which gives the most accurate results is $0.3 < \alpha < 0.4$. Again comparison purposes, we used the same values of the coefficients v_4, v_6 and v_8.

In Tables 4.9-4.12, we give the computed eigenvalues of $x^2 + v_4x^4$ with $v_4 = 0.1, 0.5,$ 1,and 5, respectively. Similarly, Tables 4.13-4.16 and Tables 4.17-4.20 present the eigenvalues for $v(x) = x^2 + v_6x^6$ and $v(x) = x^2 + v_8x^8$. Finally, in Table 4.21 we give the eigenvalues of $v(x) = x^2 + 0.5x^4 + 0.5x^6$.

Table 4.9: Eigenvalues of $v(x) = x^2 + 0.1x^4$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	0.77821814	1.04399817	1.06528551	1.06528550
	2	2.45684459	3.12158479	3.30687201	3.30687174
	3	5.23643426	5.12838578	5.74795927	5.74795585
	4	10.07118779	7.36889553	8.35267783	8.35264842
	5	17.00870826	10.46539840	11.09859562	11.09840147
$N = 35$	1	0.77868548	1.04409364	1.06528551	1.06528550
	2	2.45834074	3.12254276	3.30687201	3.30687174
	3	5.23855288	5.13178476	5.74795927	5.74795589
	4	10.07335633	7.37485171	8.35267783	8.35264880
	5	17.01087644	10.47228854	11.09859562	11.09840420

Table 4.10: Eigenvalues of $v(x) = x^2 + 0.5x^4$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.02309087	1.23833750	1.24185406	1.24185406
	2	3.15070857	4.01693537	4.05193232	4.05193233
	3	6.06399040	7.21292881	7.39690065	7.39690064
	4	10.76305278	10.51238286	11.11515495	11.1151542
	5	17.60428779	13.89268574	15.13684861	15.13684575
$N = 35$	1	1.02375162	1.23836518	1.24185406	1.24185406
	2	3.15343352	4.01724645	4.05193233	4.05193233
	3	6.06865774	7.21480925	7.39690064	7.39690064
	4	10.76827286	10.51920465	11.11515428	11.11515428
	5	17.60951629	13.90743250	15.13684575	15.13684575

Table 4.11: Eigenvalues of $v(x) = x^2 + x^4$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.24367260	1.39171573	1.39235165	1.39235164
	2	3.88803404	4.64218227	4.64881273	4.64881270
	3	7.09363103	8.61478616	8.65504716	8.65504996
	4	11.69930683	12.98363314	13.15677362	13.15680390
	5	18.39805834	17.51077974	18.05764381	18.05755743
$N = 35$	1	1.24430863	1.39172200	1.39235164	1.39235164
	2	3.89138200	4.64225389	4.64881270	4.64881270
	3	7.10071608	8.61527774	8.65504996	8.65504996
	4	11.70835141	12.98607142	13.15680390	13.15680390
	5	18.40737547	17.51954815	18.05755744	18.05755744

Table 4.12: Eigenvalues of $v(x) = x^2 + 5x^4$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	2.00513163	2.01834048	2.01833601	2.01834063
	2	6.90747928	7.01347721	7.01316949	7.01347884
	3	12.98420734	13.46771447	13.46519639	13.46772812
	4	19.39380318	20.81386615	20.81942817	20.81397885
	5	26.18319353	28.87446672	29.00067237	28.87523713
$N = 35$	1	2.00524431	2.01834049	2.01834065	2.01834065
	2	6.90848786	7.01347723	7.01347917	7.01347919
	3	12.98942369	13.46771469	13.46773099	13.46773041
	4	19.41042879	20.81386765	20.81397358	20.81396694
	5	26.21584221	28.87447521	28.87499743	28.87499635

Table 4.13: Eigenvalues of $v(x) = x^2 + 0.1x^6$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	0.82136037	1.10238525	1.10908704	1.10908708
	2	2.59735307	3.53920387	3.59603643	3.59603692
	3	5.42573191	6.39805724	6.64438870	6.64439171
	4	10.23766105	9.54297263	10.23786735	10.23787372
	5	17.14686086	12.96695958	14.30710440	14.30704008
$N = 35$	1	0.82213901	1.10246074	1.10908708	1.10908708
	2	2.59998114	3.53991470	3.59603692	3.59603692
	3	5.42963941	6.40148887	6.64439171	6.64439171
	4	10.24177732	9.55335162	10.23787372	10.23787372
	5	17.15099475	12.98735508	14.30704004	14.30704005

Table 4.14: Eigenvalues of $v(x) = x^2 + 0.5x^6$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.13401101	1.30087528	1.30097998	1.30098698
	2	3.65592681	4.46276449	4.46362876	4.46368312
	3	6.95008805	8.68182831	8.68628449	8.68639366
	4	11.67655656	13.79043508	13.80929108	13.80828453
	5	18.37785622	19.61873171	19.68933331	19.67782121
$N = 35$	1	1.13513104	1.30087729	1.30098697	1.30098697
	2	3.66132059	4.46278182	4.46368302	4.46368308
	3	6.96130429	8.68192025	8.68639364	8.68639398
	4	11.69129085	13.79082617	13.80828963	13.80829058
	5	18.39356859	19.62016800	19.67786960	19.67786640

Table 4.15: Eigenvalues of $v(x) = x^2 + x^6$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.34804349	1.43562078	1.43562823	1.43562447
	2	4.53988151	5.03336446	5.03325961	5.03339510
	3	8.58481692	9.96645826	9.96461527	9.96662356
	4	13.57703878	15.98874767	15.97578910	15.98948891
	5	20.12211425	22.90763384	22.86784451	22.91056041
$N = 35$	1	1.34888050	1.43562085	1.43562469	1.43562462
	2	4.54486603	5.03336508	5.03339666	5.03339594
	3	8.59888479	9.96646164	9.96662637	9.96662200
	4	13.60123088	15.98876274	15.98945494	15.98944078
	5	20.15213249	22.90769287	22.91016767	22.91018039

Table 4.16: Eigenvalues of $v(x) = x^2 + 5x^6$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.90917691	1.91245383	1.91128342	1.91243877
	2	6.93892856	6.96085713	6.95341081	6.96078634
	3	14.07706707	14.16909927	14.16135290	14.16930401
	4	22.73502342	23.04152650	23.19954684	23.04540916
	5	32.42847415	33.27287823	34.07590753	33.29729901
$N = 35$	1	1.90923202	1.91245383	1.91246042	1.91245381
	2	6.93931952	6.96085713	6.96092740	6.96085699
	3	14.07885754	14.16909927	14.16958004	14.16909876
	4	22.74167405	23.04152650	23.04331861	23.04152663
	5	32.44902932	33.27287825	33.27378287	33.27289621

Table 4.17: Eigenvalues of $v(x) = x^2 + 0.1x^8$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	0.90040430	1.16859413	1.16899756	1.16897047
	2	2.86499847	3.93694361	3.93990939	3.93972209
	3	5.81131004	7.62832557	7.64054004	7.63995660
	4	10.60557592	12.24339256	12.28114575	12.28121949
	5	17.46496405	17.65575703	17.74989850	17.76146648
$N = 35$	1	0.90189675	1.16860327	1.16897056	1.16897045
	2	2.87053538	3.93701397	3.93972209	3.93972136
	3	5.82033292	7.62863760	7.63995081	7.63994849
	4	10.61569369	12.24448754	12.28116835	12.28116774
	5	17.47530759	17.65911714	17.76117289	17.76121363

Table 4.18: Eigenvalues of $v(x) = x^2 + 0.5x^8$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.27068045	1.36772091	1.36730379	1.36772304
	2	4.32623525	4.83915528	4.83569944	4.83918737
	3	8.39140286	9.77735896	9.76077899	9.77762384
	4	13.56884494	16.07135190	16.01521855	16.07276426
	5	20.24815427	23.54080303	23.45085108	23.54668226
$N = 35$	1	1.27204127	1.36772091	1.36772607	1.36772102
	2	4.33370369	4.83915530	4.83918848	4.83915602
	3	8.41150873	9.77735907	9.77747487	9.77736201
	4	13.60378548	16.07135231	16.07153627	16.07136178
	5	20.29345285	23.54080440	23.54014941	23.54082998

Table 4.19: Eigenvalues of $v(x) = x^2 + x^8$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.45443154	1.49101990	1.49164297	1.49097978
	2	5.16194558	5.36877806	5.37097110	5.36846606
	3	10.33082783	10.99373732	10.98828972	10.99224891
	4	16.63046206	18.19109998	18.09571790	18.18568101
	5	23.91095664	26.74344855	26.27554829	26.73006112
$N = 35$	1	1.45510986	1.49101990	1.49100936	1.49101978
	2	5.16602825	5.36877806	5.36873050	5.36877730
	3	10.34482556	10.99373733	10.99374600	10.99373476
	4	16.66484594	18.19110000	18.19210062	18.19109499
	5	23.97352728	26.74344850	26.75085878	26.74345735

Table 4.20: Eigenvalues of $v(x) = x^2 + 5x^8$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.88703727	1.88748718	1.88160102	1.88719192
	2	7.00825824	7.01093079	6.98460727	7.00966632
	3	14.66930090	14.67927283	14.67627429	14.67948901
	4	24.51315063	24.54408093	24.88139816	24.56795683
	5	36.20185978	36.28724570	38.12924093	36.44855707
$N = 35$	1	1.88704900	1.88748714	1.88770418	1.88748206
	2	7.00833002	7.01093057	7.01255689	7.01089533
	3	14.66958128	14.67927222	14.68746710	14.67911762
	4	24.51407592	24.54408081	24.57308431	24.54354400
	5	36.20462164	36.28725536	36.35470965	36.28593542

Table 4.21: Eigenvalues of $v(x) = x^2 + 0.5x^4 + 0.5x^6$ with Chebyshev pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.30743353	1.42128573	1.42131617	1.42132032
	2	4.26525578	4.89125318	4.89149307	4.89155938
	3	7.90152362	9.48052429	9.48166824	9.48219095
	4	12.65032696	14.95874214	14.96372917	14.96584516
	5	19.23336496	21.17282175	21.20041884	21.19829919
$N = 35$	1	1.30826754	1.42128633	1.42132031	1.42132031
	2	4.27002955	4.89125874	4.89155922	4.89155923
	3	7.91342206	9.48055647	9.48218947	9.48218970
	4	12.66810772	14.95889032	14.96583740	14.96583969
	5	19.25334706	21.17340646	21.19828276	21.19829608

4.4 Eigenvalues of Schrödinger equation via Legendre pseudospectral method

Finally, we applied the Legendre pseudospectral formulation for the Schrödinger equation with polynomial potential which to our knowledge has not been considered before. The substitution transforming the infinite interval $(-\infty, \infty)$ to $[-1, 1]$ used in our study is

$$t = \tanh(\alpha x), \tag{4.3}$$

where $\alpha > 0$ is an optimization parameter. As in Chebyshev scheme, we tried various values for α and we observed that the most accurate results with the same N are obtained when $0.3 < \alpha < 0.4$.

In Tables 4.22-4.25 we give the computed eigenvalues of $x^2 + v_4x^4$ with $v_4 = 0.1, 0.5$, 1, and 5 respectively. Similarly, Tables 4.26-4.29 and Tables 4.30-4.33 present the eigenvalues for $v(x) = x^2 + v_6x^6$ and $v(x) = x^2 + v_8x^8$. Finally, in Table 4.34, we give the eigenvalues of $v(x) = x^2 + 0.5x^4 + 0.5x^6$.

Table 4.22: Eigenvalues of $v(x) = x^2 + 0.1x^4$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.06523087	1.06528566	1.06528551	1.06528551
	2	3.30572422	3.30686877	3.30687201	3.30687201
	3	5.73925266	5.74786786	5.74795909	5.74795902
	4	8.32476701	8.35189756	8.35267668	8.35267552
	5	11.09039221	11.09577238	11.09860131	11.09859147
$N = 35$	1	1.06528779	1.06528551	1.06528551	1.06528551
	2	3.30685123	3.30687212	3.30687201	3.30687201
	3	5.74717374	5.74796181	5.74795927	5.74795927
	4	8.34540267	8.35269802	8.35267783	8.35267782
	5	11.06534188	11.09864403	11.09859563	11.09859559

Table 4.23: Eigenvalues of $v(x) = x^2 + 0.5x^4$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.24185735	1.24185393	1.24185410	1.24185406
	2	4.05208372	4.05192891	4.05193269	4.05193243
	3	7.39840069	7.39686461	7.39689779	7.39690133
	4	11.12095630	11.11497275	11.11508482	11.11515246
	5	15.13418074	15.13662411	15.13653242	15.13678982
$N = 35$	1	1.24185245	1.24185406	1.24185406	1.24185406
	2	4.05191097	4.05193232	4.05193233	4.05193233
	3	7.39677208	7.39690076	7.39690064	7.39690064
	4	11.11487073	11.11515666	11.11515429	11.11515427
	5	15.13808820	15.13686273	15.13684588	15.13684572

Table 4.24: Eigenvalues of $v(x) = x^2 + x^4$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.39233946	1.39235167	1.39235128	1.39235164
	2	4.64866785	4.64881400	4.64880867	4.64881250
	3	8.65427283	8.65506588	8.65505802	8.65504682
	4	13.15550075	13.15688906	13.15717124	13.15678589
	5	18.06573383	18.05762882	18.05920876	18.05757240
$N = 35$	1	1.39235199	1.39235164	1.39235164	1.39235164
	2	4.64881618	4.64881272	4.64881270	4.64881270
	3	8.65505865	8.65505004	8.65504997	8.65504996
	4	13.15669679	13.15680389	13.15680402	13.15680389
	5	18.05630541	18.05755331	18.05755764	18.05755742

Table 4.25: Eigenvalues of $v(x) = x^2 + 5x^4$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	2.01833959	2.01834062	2.01828991	2.01834071
	2	7.01346291	7.01347848	7.01291597	7.01348552
	3	13.46760044	13.46772283	13.46822754	13.46781824
	4	20.81342486	20.81392695	20.84355093	20.81423059
	5	28.87454546	28.87495551	28.92968083	28.87251179
$N = 35$	1	2.01834064	2.01834065	2.01834069	2.01834065
	2	7.01347914	7.01347919	7.01347971	7.01347919
	3	13.46773091	13.46773042	13.46773250	13.46773042
	4	20.81397517	20.81396691	20.81393729	20.81396676
	5	28.87505117	28.87499575	28.87466289	28.87499442

Table 4.26: Eigenvalues of $v(x) = x^2 + 0.1x^6$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.10913158	1.10908502	1.10908493	1.10908741
	2	3.59673752	3.59600379	3.59600962	3.59603941
	3	6.64912266	6.64413326	6.64423837	6.64439256
	4	10.25553004	10.23660227	10.23755840	10.23776622
	5	14.33495987	14.30308482	14.30905999	14.30612198
$N = 35$	1	1.10907701	1.10908700	1.10908708	1.10908708
	2	3.59592271	3.59603604	3.59603697	3.59603692
	3	6.64373424	6.64438674	6.64439222	6.64439168
	4	10.23548559	10.23785751	10.23787711	10.23787326
	5	14.30209050	14.30702767	14.30705410	14.30703642

Table 4.27: Eigenvalues of $v(x) = x^2 + 0.5x^6$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.30101157	1.30098487	1.30094903	1.30099106
	2	4.46377763	4.46365743	4.46345804	4.46371489
	3	8.68599946	8.68621735	8.68654362	8.68649709
	4	13.80237016	13.80745815	13.81633257	13.80808626
	5	19.64434943	19.67526312	19.72942694	19.67376668
$N = 35$	1	1.30098439	1.30098699	1.30098672	1.30098696
	2	4.46366159	4.46368312	4.46368061	4.46368299
	3	8.68629610	8.68639361	8.68638116	8.68639371
	4	13.80801819	13.80828516	13.80825618	13.80829124
	5	19.67766771	19.67782942	19.67794526	19.67787986

Table 4.28: Eigenvalues of $v(x) = x^2 + x^6$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.43562558	1.43562665	1.43558113	1.43561421
	2	5.03347855	5.03341847	5.03247659	5.03333064
	3	9.96748576	9.96676802	9.95858376	9.96653816
	4	15.99435165	15.99007229	15.95052610	15.99069217
	5	22.92784888	22.91182210	22.84082832	22.92124380
$N = 35$	1	1.43562563	1.43562459	1.43562568	1.43562466
	2	5.03340355	5.03339571	5.03340564	5.03339632
	3	9.96665256	9.96662090	9.96667250	9.96662421
	4	15.98949774	15.98943761	15.98955950	15.98944883
	5	22.90999893	22.91017951	22.90978486	22.91018978

Table 4.29: Eigenvalues of $v(x) = x^2 + 5x^6$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.91245513	1.91245170	1.91085538	1.91238806
	2	6.96089620	6.96085135	6.95314702	6.96070105
	3	14.16947735	14.16915638	14.18357771	14.17155146
	4	23.04369447	23.04218343	23.31496132	23.06414338
	5	33.28107701	33.27651751	34.26916982	33.37039412
$N = 35$	1	1.91245379	1.91245385	1.91248042	1.91245304
	2	6.96085722	6.96085731	6.96109653	6.96085129
	3	14.16910270	14.16910032	14.17040873	14.16907771
	4	23.04155561	23.04153102	23.04489094	23.04151125
	5	33.27303422	33.27289115	33.26561440	33.27331610

Table 4.30: Eigenvalues of $v(x) = x^2 + 0.1x^8$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.16881854	1.16894504	1.16913690	1.16894127
	2	3.93821953	3.93954215	3.94098877	3.93945483
	3	7.63178440	7.63931101	7.64485274	7.63859306
	4	12.24915931	12.27990343	12.28950933	12.27622222
	5	17.66611997	17.76167021	17.73603399	17.74875867
$N = 35$	1	1.16896057	1.16896998	1.16897315	1.16897080
	2	3.93966773	3.93971690	3.93974585	3.93972436
	3	7.63985744	7.63992409	7.64007691	7.63996323
	4	12.28152126	12.28106528	12.28164349	12.28122019
	5	17.76457982	17.76086264	17.76247695	17.76135008

Table 4.31: Eigenvalues of $v(x) = x^2 + 0.5x^8$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.36758291	1.36770765	1.36669658	1.36759181
	2	4.83837763	4.83910778	4.83073520	4.83843782
	3	9.77522449	9.77744286	9.73789395	9.77582362
	4	16.06923782	16.07286966	15.94474052	16.07336873
	5	23.55226472	23.54943882	23.33327888	23.57675792
$N = 35$	1	1.36772015	1.36772130	1.36775242	1.36772180
	2	4.83915819	4.83915746	4.83937573	4.83916443
	3	9.77741975	9.77736451	9.77826143	9.77741778
	4	16.07176242	16.07135183	16.07372208	16.07163204
	5	23.54267728	23.54072264	23.54294310	23.54188929

Table 4.32: Eigenvalues of $v(x) = x^2 + x^8$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.49097356	1.49099990	1.49216006	1.49086529
	2	5.36831059	5.36859394	5.37213067	5.36724388
	3	10.99095419	10.99269485	10.97822409	10.98468049
	4	18.17871483	18.18655610	18.00542654	18.15180974
	5	26.70030474	26.72776414	25.93402071	26.62129447
$N = 35$	1	1.49101798	1.49101937	1.49096002	1.49101644
	2	5.36876016	5.36877492	5.36845373	5.36874817
	3	10.99363375	10.99372721	10.99308585	10.99357409
	4	18.19062967	18.19108164	18.19227448	18.19039319
	5	26.74169159	26.74346810	26.76228292	26.74099783

Table 4.33: Eigenvalues of $v(x) = x^2 + 5x^8$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.88737455	1.88741166	1.88052064	1.88631521
	2	7.01018966	7.01039653	6.98416575	7.00541507
	3	14.67622047	14.67686412	14.70828891	14.67272087
	4	24.53428274	24.53553738	25.04460675	24.58737554
	5	36.26315566	36.26394106	38.93640760	36.64593094
$N = 35$	1	1.88748848	1.88748652	1.88791810	1.88746088
	2	7.01093701	7.01092571	7.01413864	7.01071889
	3	14.67928516	14.67924688	14.69506790	14.67816555
	4	24.54405987	24.54397213	24.59775636	24.53947908
	5	36.28693355	36.28686318	36.40150930	36.27237435

Table 4.34: Eigenvalues of $v(x) = x^2 + 0.5x^4 + 0.5x^6$ with Legendre pseudospectral method

N	i	$E_i(\alpha = 1)$	$E_i(\alpha = 0.7)$	$E_i(\alpha = 0.3)$	$E_i(\alpha = 0.4)$
$N = 25$	1	1.42134433	1.42132099	1.42128451	1.42132184
	2	4.89175756	4.89156072	4.89115042	4.89158220
	3	9.48296935	9.48215624	9.47997063	9.48237516
	4	14.96661379	14.96545623	14.96159747	14.96665519
	5	21.18838565	21.19607886	21.22963264	21.19947269
$N = 35$	1	1.42131948	1.42132033	1.42132031	1.42132031
	2	4.89154964	4.89155936	4.89155855	4.89155916
	3	9.48212543	9.48219047	9.48218038	9.48218915
	4	14.96553853	14.96584236	14.96576979	14.96583671
	5	21.19732047	21.19829827	21.19798960	21.19828625

4.5 Comparison of the four pseudospectral methods

In this last Section, we compare the results obtained by using the four different psedospectral schemes. The Tables 4.35-4.44 show the eigenvalues for each choice of the parameters v_i in the potential obtained with the Hermite, Laguerre, Chebyshev and Legendre methods.

The numerical evidence presented in the tables above show that the Chebyshev and Legendre pseudospectral methods can be as efficient as the Hermite and Laguerre schemes for the Schrödinger equation with polynomial potential. Although the use of Chebyshev or Legendre polynomials requires transformation of the originally infinite interval to a finite one, and therefore has not been considered until now, our calculations show that these two types of orthogonal polynomials are also good candidate for the application of pseudospectral methods for various types of differential equations on both finite and infinite intervals of the independent variable.

Table 4.35: Eigenvalues for the potential $v(x) = x^2 + 0.1x^4$ with all pseudospectral methods

Hermite ($N = 25$)	Laguerre ($N = 25$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.3$)
1.06528551	1.06528551	1.06528551	1.06528551
3.30687201	3.30687201	3.30687201	3.30687201
5.74795927	5.74795927	5.74795927	5.74795927
8.35267783	8.35267783	8.35267783	8.35267783
11.09859562	11.09859562	11.09859562	11.09859563

Table 4.36: Eigenvalues for the potential $v(x) = x^2 + x^4$ with all pseudospectral methods

Hermite ($N = 30$)	Laguerre ($N = 30$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.4$)
1.39235165	1.39235164	1.39235164	1.39235164
4.64881285	4.64881270	4.64881270	4.64881270
8.65505068	8.65504996	8.65504996	8.65504996
13.15679328	13.15680390	13.15680390	13.15680389
18.05742404	18.05755744	18.05755744	18.05755742

Table 4.37: Eigenvalues for the potential $v(x) = x^2 + 5x^4$ with all pseudospectral methods

Hermite ($N = 35$)	Laguerre ($N = 35$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.4$)
2.01833982	2.01834065	2.01834065	2.01834065
7.01349181	7.01347918	7.01347918	7.01347919
13.46807428	13.46773043	13.46773099	13.46773042
20.81471332	20.81396696	20.81397358	20.81396676
28.85976412	28.87499529	28.87499743	28.87499442

Table 4.38: Eigenvalues for the potential $v(x) = x^2 + 0.1x^6$ with all pseudospectral methods

Hermite ($N = 25$)	Laguerre ($N = 25$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.3$)
1.10908716	1.10908708	1.10908708	1.10908708
3.59603630	3.59603692	3.59603692	3.59603697
6.64437193	6.64439171	6.64439171	6.64439222
10.23768356	10.23787374	10.23787372	10.23787711
14.30611359	14.30703992	14.30704004	14.30705410

Table 4.39: Eigenvalues for the potential $v(x) = x^2 + x^6$ with all pseudospectral methods

Hermite ($N = 30$)	Laguerre ($N = 30$)	Chebyshev ($N = 35, \alpha = 0.4$)	Legendre ($N = 35, \alpha = 0.4$)
1.43564880	1.43562462	1.43562462	1.43562466
5.03367987	5.03339576	5.03339594	5.03339632
9.96821797	9.96662340	9.96662200	9.96662421
15.99379401	15.98943017	15.98944078	15.98944883
22.89545417	22.91023711	22.91018039	22.91018978

Table 4.40: Eigenvalues for the potential $v(x) = x^2 + 5x^6$ with all pseudospectral methods

Hermite ($N = 35$)	Laguerre ($N = 35$)	Chebyshev ($N = 35, \alpha = 0.4$)	Legendre ($N = 35, \alpha = 0.4$)
1.91276328	1.91245485	1.91245382	1.91245304
6.96336437	6.96085056	6.96085699	6.96085129
14.18003443	14.16913161	14.16909876	14.16907771
23.04370562	23.04155096	23.04152663	23.04151125
33.01059877	33.27203775	33.27289621	33.27331610

Table 4.41: Eigenvalues for the potential $v(x) = x^2 + 0.1x^8$ with all pseudospectral methods

Hermite ($N = 25$)	Laguerre ($N = 25$)	Chebyshev ($N = 35, \alpha = 0.4$)	Legendre ($N = 35, \alpha = 0.4$)
1.16900468	1.16897037	1.16897045	1.16897080
3.94016015	3.93972374	3.93972136	3.93972436
7.64315281	7.63993455	7.63994849	7.63996323
12.29573841	12.28124256	12.28116774	12.28122019
17.80727064	17.76083613	17.76121363	17.76135008

Table 4.42: Eigenvalues for the potential $v(x) = x^2 + x^8$ with all pseudospectral methods

Hermite ($N = 30$)	Laguerre ($N = 30$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.4$)
1.49119533	1.49100746	1.49100936	1.49101644
5.37183136	5.36885449	5.36873050	5.36874817
11.01461166	10.99329709	10.99374600	10.99357409
18.29386579	18.19207670	18.19210062	18.19039319
27.01871881	26.73943454	26.75085878	26.74099783

Table 4.43: Eigenvalues for the potential $v(x) = x^2 + 5x^8$ with all pseudospectral methods

Hermite ($N = 35$)	Laguerre ($N = 35$)	Chebyshev ($N = 35, \alpha = 0.4$)	Legendre ($N = 35, \alpha = 0.4$)
1.89065515	1.88755248	1.88748206	1.88746088
7.02984538	7.01050971	7.01089533	7.01071889
14.74110874	14.68100653	14.67911762	14.67816555
24.59300359	24.54000270	24.54354400	24.53947908
35.72589754	36.29275834	36.28593542	36.27237435

Table 4.44: Eigenvalues for the potential $v(x) = x^2 + 0.5x^4 + 0.5x^6$ with all pseudospectral methods

Hermite ($N = 25$)	Laguerre ($N = 25$)	Chebyshev ($N = 35, \alpha = 0.3$)	Legendre ($N = 35, \alpha = 0.4$)
1.42133242	1.42132029	1.42132031	1.42132031
4.89157673	4.89155939	4.89155922	4.89155916
9.48129007	9.48218802	9.48218947	9.48218915
14.95600331	14.96584081	14.96583740	14.96583671
21.15764505	21.19830062	21.19828276	21.19828625

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APPENDIX A

MATLAB CODES

A.1 Matlab code for Hermite Pseudospectral method

The following is a MATLAB code which computes the eigenvalues of the Schrödinger equation with polynomial potential using Hermite pseudospectral method.

```
% THIS PROGRAM USES HERMITE PSEUDOSPECTRAL METHOD
%First part: input of the parameters
clc
clear all
N=input('Truncation Order');
alp=input('Parameter v4');
bet=input('Parameter v6');
gam=input('Parameter v8');
R=zeros(N,N);
B=zeros(N,N);
%Entries of the matrix R
R(N,N)=0;
for i=1:N-1
    R(i,i)=0;
    R(i,i+1)=-sqrt(i/2);
end
for i=2:N
    R(i,i-1)=-sqrt((i-1)/2);
end
```

```
%Eigenvalues of R(Zeros of Hermite polynomials)
[v,D]=eig(R);
for i=1:N
 tu(i)=D(i,i);
end
t=sort(tu)
%The values of polynomial potential v(x) at the nodes
for i=1:N
 v(i)=(t(i))^2+alp*(t(i))^4+bet*(t(i))^6+gam*(t(i))^8;
end
% Construction of the matrix P
for i=1:N
    B(i,i)=(2/3)*(t(i)*t(i)+N-1)+(v(i)-t(i)*t(i));
    for j=i+1:N
        B(i,j)=2/((t(i)-t(j))*(t(i)-t(j)));
    end
    for j=1:i-1
        B(i,j)=2/((t(i)-t(j))^2);
    end
end
% Eigenvalues of the problem
[Y,L]=eig(B);
for i=1:N
 e(i)=L(i,i)+1;
end
fileID=fopen('herm1.txt','w')
for i=1:N
    fprintf(fileID,'%3d %10.8f n', i-1, e(i))
end
fclose(fileID)
```

A.2 Matlab code for Laguerre Pseudospectral method

The following is a MATLAB code which computes the eigenvalues of the Schrödinger equation with polynomial potential using Laguerre pseudospectral method.

```
%THIS PROGRAM USES LAGUERRE PSEUDOSPECTRAL METHOD
%First part: input of the parameters
clc
clear all
alp=input('Order of Associated Laguerre Polynomial');
q1=input('Parameter v4');
q2=input('Parameter v6');
q3=input('Parameter v8');
N=input('Truncation Order');
R=zeros(N,N);
u=zeros(N);
w=zeros(N);
%Entries of the matrix R
R(N,N)=alp+2*N-1;
for i=1:N-1
    R(i,i)=alp+2*i-1;
    R(i,i+1)=-sqrt(i*(alp+i));
end
for i=2:N
    R(i,i-1)=-sqrt((i-1)*(alp+i-1));
end
%Eigenvalues of R(Zeros of Laguerre polynomials)
[v,D]=eig(R);
for i=1:N
 tu(i)=D(i,i);
end
t=sort(tu)
%The values of polynomial potential v(x) at the nodes
```

```
for i=1:N
    u(i)=t(i)+q1*(t(i))^2+q2*(t(i)^3)+q3*(t(i)^4);
    w(i)=0.25*t(i)-0.25*u(i)-0.5*(alp+1);
end
% Construction of the matrix P

for i=1:N
    B(i,i)=-(1/(6*t(i)))*(alp-1-t(i))*(alp+1-t(i))-((N-1)/3)+w(i);
    for j=i+1:N
        B(i,j)=-(2*sqrt(t(i)*t(j)))/((t(i)-t(j))*(t(i)-t(j)));
    end
    for j=1:i-1
        B(i,j)=-(2*sqrt(t(i)*t(j)))/((t(i)-t(j))*(t(i)-t(j)));
    end
end
% Eigenvalues of the problem
[Y,L]=eig(B);
for i=1:N
 e(i)=-4*L(i,i);
end
gi=sort(e)
[gi']
fileID=fopen('lag1.txt','w')
for i=1:N
    fprintf(fileID,'%3d %10.8f n', i-1, gi(i))
end
fclose(fileID)
```

A.3 Matlab code for Chebyshev Pseudospectral method

The following is a MATLAB code which computes the eigenvalues of the Schrödinger equation with polynomial potential using Chebyshev pseudospectral method.

```
%THIS PROGRAM USES CHEBYSHEV PSEUDOSPECTRAL METHOD
%First part: input of the parameters
clc
clear all
alp=input('Optimization parameter');
q1=input('Parameter v4');
q2=input('Parameter v6');
q3=input('Parameter v8');
N=input('Truncation Order');
R=zeros(N,N);
R(N,N)=0;
R(1,2)=1;
R(1,1)=0;
p=zeros(N);
z=zeros(N);
x=zeros(N);
v=zeros(N);
w=zeros(N);
for i=1:N
    p(i)=cos((pi*(i-0.5))/N);
end
for i=2:N-1
    R(i,i)=0;
    R(i,i+1)=0.5;
end
for i=2:N
    R(i,i-1)=0.5;
end
%Eigenvalues of R(Zeros of chebyshev polynomials)
[v,D]=eig(R);
for i=1:N
 tu(i)=D(i,i);
```

```
end
t=sort(tu)
for i=1:N
    s=t(i);
    x(i)=(1/alp)*asin(s);
end
%The values of polynomial potential v(x) at the nodes
for i=1:N
    v(i)=(1/(alp^2))*(x(i)^2+q1*(x(i))^4+q2*(x(i))^6+q3*(x(i))^8);
    w(i)=1-t(i)^2;
end
% Construction of the matrix P
for i=1:N
    B(i,i)=(0.5*(t(i)^2))/w(i)-(N^2-1)/3-v(i);
    for j=i+1:N
        B(i,j)=-(2*sqrt(w(i)*w(j)))/((t(i)-t(j))^2);
    end
    for j=1:i-1
        B(i,j)=-(2*sqrt(w(i)*w(j)))/((t(i)-t(j))^2);
    end
end
% Eigenvalues of the problem
[Y,L]=eig(B);
for i=1:N
 e(i)=-(alp^2)*L(i,i);
end
gi=sort(e)
fileID=fopen('cheby5.txt','w')
for i=1:N
    fprintf(fileID,'%3d %10.8f n', i-1,  e(i))
end
fclose(fileID)
```

A.4 Matlab code for Legendre Pseudospectral method

The following is a MATLAB code which computes the eigenvalues of the Schrödinger equation with polynomial potential using Legendre pseudospectral method.

```
%THIS PROGRAM USES LEGENDRE PSEUDOSPECTRAL METHOD
%First part: input of the parameters
clc
clear all
alp=input('Optimization parameter');
q1=input('Parameter v4');
q2=input('Parameter v6');
q3=input('Parameter v8');
N=input('Truncation Order');
R=zeros(N,N);
%Entries of the matrix R
R(N,N)=0;
for i=1:N-1
    R(i,i)=0;
    R(i,i+1)=i/sqrt((2*i-1)*(2*i+1));
end
for i=2:N
    R(i,i-1)=(i-1)/sqrt((2*i-3)*(2*i-1));
end
%Eigenvalues of R(Zeros of Legendre polynomials)
[v,D]=eig(R);
for i=1:N
 tu(i)=D(i,i);
end
t=sort(tu)
%The values of polynomial potential v(x) at the nodes
for i=1:N
```

```
    x(i)=(1/alp)*0.5*log((1+t(i))/(1-t(i)));
     v(i)=(1/(alp^2))*(x(i)^2+q1*(x(i))^4+q2*(x(i))^6+q3*(x(i))^8);
    w(i)=1-(t(i))^2
end
% Construction of the matrix P


for i=1:N
    B(i,i)=(2/3)*t(i)*t(i)-((N-1)*(N+2)*(1-(t(i))^2))/3-v(i);
    for j=i+1:N
        B(i,j)=-(2*w(i)*w(j))/((t(i)-t(j))*(t(i)-t(j)));
    end
    for j=1:i-1
        B(i,j)=-(2*w(i)*w(j))/((t(i)-t(j))*(t(i)-t(j)));
    end
end
% Eigenvalues of the problem
[Y,L]=eig(B);
for i=1:N
 e(i)=-alp^2*L(i,i);
end
gi=sort(e)
fileID=fopen('legen3.txt','w')
for i=1:N
    fprintf(fileID,'%3d %10.8f n', i-1,  e(i))
end
fclose(fileID)
```

VITA

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FOREIGN LANGUAGES

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