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Anharmonic oscillator via Legendre and Chebyshev pseudo-spectral methods

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Abstract

In this study, we introduce the pseudospectral methods based on Chebyshev and Legendre polynomials for the Schrödinger equation of anharmonic oscillator. The method transforms the problem into an unsymmetric matrix eigenvalue problem which can be symmetrized by using a suitable similarity transformation. Computation of the zeros of the relevant orthogonal polynomials is also converted into a symmetric matrix eigenvalue problem. The method is applied to the Scrödinger equation of an anharmonic oscillator of various types and the numerical results and discussed.

Keywords: Schrödinger equation, pseudospectral method, Chebyshev polynomial, Legendre polynomial
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1. Introduction

One of the most simple looking, but most extensively studied problems in quantum mechanics is the problem of finding the eigenvalues of the so called anharmonic oscillator. The simplicity of the Schrödinger equation for a one dimensional anharmonic oscillator does not imply that it can be solved easily. For many years, numerous studies based on different numerical methods on this problem have been reported [2, 3, 4, 5].

The pseudospecral methods have been proved to be very efficient and powerful for numerical solutions of both ordinary and partial differential equations. The construction of the pseudospectral methods employs the Lagrange interpolation with nodes chosen as the zeros of some orthogonal polynomial. As a result, the relevant boundary or eigenvalue problem for the differential equation is transformed into an unsymmetric

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matrix eigenvalue problem. However, using a suitable similarity transformation, it can be converted into a symmetric eigenvalue problem [6, 7, 8, 9, 10].

The paper is organized as follows. In the next section, we introduce briefly the general formulation of the pseudospectral methods. In Section 3, the computation of the zeros of Chebyshev and Legendre polynomials is derived. The next two sections present the application of Chebyshev and Legendre pseudospectral methods to the Schrödinger equation of a one dimensional anharmonic oscillator. The numerical results are presented in Section 6 and conclusion and some remarks are given in Section 7.

2. Formulation of the Pseudospectral Methods

The formulation of the pseudospectral methods is based on the Lagrange interpolating polynomial which interpolates a function $y = f(x)$ at the nodes (x_n, y_n) $n = 0, 1, \ldots, N$ and has the form

$$L(x) = \sum_{n=0}^{N} \ell_n(x) y_n, \quad y_n = f(x_n), \quad n = 0, \ldots, N, \tag{1}$$

where

$$\ell_n(x) = \frac{\prod_{m=0, m\neq n}^{N} (x - x_m)}{\prod_{m=0, m\neq n}^{N} (x_n - x_m)}. \tag{2}$$

Using the notation

$$F_{N+1}(x) = (x - x_0) \cdots (x - x_n) \cdots (x - x_N), \tag{3}$$

and the immediate fact that

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

we can write the polynomials $\ell_n(x)$ in (2) as

$$\ell_n(x) = \begin{cases} \dfrac{F_{N+1}(x)}{(x - x_n) F'_{N+1}(x_n)} & \text{if} \quad x \neq x_n \\ 1 & \text{if} \quad x = x_n \end{cases}. \tag{4}$$

Since any orthogonal polynomial of degree N has exactly N real and distinct zeros, then it can be written as

$$F_N(x) = a_N (x - x_0)(x - x_1) \cdots (x - x_{N-1}). \tag{5}$$

Therefore, if we take the function F_{N+1} in (4) as an orthogonal polynomial then the points $x_0, \ldots, x_N$ will be the real distinct zeros of this polynomial.

3. Computation of the zeros of orthogonal polynomials

In this section, we discuss the computation of zeros $x_0, x_1, \ldots, x_N$ of any orthogonal polynomial $F_{N+1}(x)$. We employ the three-term recurrence relation of an orthogonal polynomial given in general as [1],

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

for $n \in \mathbb{N}$ where $\alpha_n, \beta_n, \gamma_n$ are constants.

Assuming that $F_{-1}(x) \equiv 0$, we write this relation for $n = 0, 1, \ldots, N$ which leads to a system of the form

$$\begin{aligned} \beta_0 F_0(x) + \alpha_0 F_1(x) &= xF_0(x), \\ \gamma_1 F_0(x) + \beta_1 F_1(x) + \alpha_1 F_2(x) &= xF_1(x), \\ \vdots \quad & \quad \vdots \\ \gamma_N F_{N-1}(x) + \beta_N F_N(x) + \alpha_N F_{N+1}(x) &= xF_N(x). \end{aligned} \tag{6}$$

In matrix form, this system is written as

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

The requirement $F_{N+1}(x) = 0$ results in a matrix eigenvalue problem of the form

$$RF = xF, \tag{7}$$

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 (7) into a symmetric one. Indeed, let

$$G = \text{diag}\{g_0, g_1, \ldots, g_N\}, \tag{8}$$

be a nonsingular diagonal matrix. Define

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

Then

$$RGY = RF = xF = xGY,$$

and hence,

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

This can be written as

$$SY = xY,$$

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

$$s_{ij} = \frac{1}{g_i} r_{ij} g_j, \quad i, j = 1, \ldots N,$$

and moreover, S is also tridiagonal, that is,

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

If we require that S is symmetric, that is,

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

then,

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

which yields

$$g_{i+1} = g_i \sqrt{\frac{\gamma_{i+1}}{\alpha_i}}, \quad i = 0, 1, \ldots, N-1. \tag{9}$$

From this equation we compute the entries g_i of the diagonal matrix G recursively, starting with some arbitrary $g_0 \neq 0$.

3.1. 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]

$$x_n = \cos\left(\frac{\pi(n+1/2)}{N+1}\right), \quad n = 0, 1, \ldots, N. \tag{10}$$

However, using the procedure described above, these zeros can also be obtained as matrix eigenvalues. The recurrence relation for Chebyshev polynomials is [1]

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

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 (7) has the form

$$R = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & 0 & \cdots & 0 \\ 0 & 1/2 & 0 & 1/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1/2 \\ 0 & 0 & 0 & \cdots & 1/2 & 0 \end{bmatrix}. \tag{11}$$

The entries of the similarity transformation matrix G are now obtained from (9) as

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

starting with $g_0 = 1$. Thus, the zeros of the Chebyshev polynomial T_{N+1} are obtained as the eigenvalues of the symmetric matrix

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

3.2. Zeros of Legendre polynomials

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

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x). \tag{12}$$

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

$$R = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & 0 & \cdots & 0 \\ 0 & \frac{2}{5} & 0 & \frac{3}{5} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \frac{N+1}{2N+1} \\ 0 & 0 & 0 & \cdots & \frac{N}{2N+1} & 0 \end{bmatrix}. \tag{13}$$

The entries of the diagonal matrix G are now obtained from (9) 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

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

4. Computation of derivatives

The pseudospectral method will be used to solve numerically the Schrödinger equation which is an ordinary differential equation of second order. The dependent variable in the equation will be approximated by its Lagrange interpolating polynomial at the nodes taken as the zeros of a suitable orthogonal polynonmial. Therefore, the derivatives of the dependent variable up to second order will also be needed.

Let

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

where

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

Then

$$y'(x) = \sum_{n=0}^{N} y_n \ell'_n(x) \quad \text{and} \quad y''(x) = \sum_{n=0}^{N} y_n \ell''_n(x).$$

Therefore, we need to compute the derivatives $\ell'_n(x)$ and $\ell''_n(x)$. First, we compute

$$\ell'_n(x) = \begin{cases} \dfrac{F'_{N+1}(x)(x-x_n) - F_{N+1}(x)}{(x-x_n)^2 F'_{N+1}(x_n)} & if \quad x \neq x_n \\ \\ \dfrac{F''_{N+1}(x_n)}{2F'_{N+1}(x_n)} & if \quad x = x_n. \end{cases}$$

Similarly, a long but straightforward computation gives the second order derivative as

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

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

$$\ell_n(x_m) = \delta_{mn} = \begin{cases} 0 & \text{if} \quad m \neq n \\ 1 & \text{if} \quad m = n, \end{cases} \tag{14}$$

$$\ell_n'(x_m) = \begin{cases} \dfrac{1}{(x_m - x_n)} \dfrac{F_{N+1}'(x_m)}{F_{N+1}'(x_n)} & if \quad m \neq n \\ \dfrac{1}{2}\dfrac{F_{N+1}''(x_n)}{F_{N+1}'(x_n)} & if \quad m = n, \end{cases} \tag{15}$$

$$\ell_n''(x_m) = \begin{cases} \dfrac{F_{N+1}''(x_m)}{(x_m - x_n)F_{N+1}'(x_n)} - \dfrac{2F_{N+1}'(x_m)}{(x_m - x_n)^2 F_{N+1}'(x_n)} & if \quad m \neq n \\ \dfrac{1}{3}\dfrac{F_{N+1}'''(x_n)}{F_{N+1}'(x_n)} & if \quad m = n. \end{cases} \tag{16}$$

5. Chebyshev and Legendre pseudospectral formulations of the Schrödinger equation

Consider the Schrödinger equation for an anharmonic oscillator.

$$\left[-\frac{d^2}{dx^2} + v(x)\right]\psi(x) = E\psi(x), \quad x \in (-\infty, \infty), \tag{17}$$

where $v(x)$ is the potential which will be assumed to be a polynomial, in general. In the numerical calculations it will be taken as a polynomial containing only positive even powers of x. The Schrödinger equation for anharmonic oscillator is defined on the whole real line. However, both Chebyshev and Legendre polynomials are orthogonal on the finite interval $[-1, 1]$. Therefore, first we need a variable transformation to transform the infinite interval $(-\infty, \infty)$ to the finite interval $[-1, 1]$.

5.1. Chebyshev pseudospectral formulation

First, we use the pseudospectral method with Chebyshev polynomials. The differential equation of Chebyshev polynomials is [1]

$$(1 - t^2)T_n''(t) - tT_n'(t) + n^2 T_n(t) = 0. \tag{18}$$

In order to transform the infinite interval to the finite interval $[-1, 1]$, and the differential operator in (17) into the form in (18), we propose the following substitution on the independent variable.

$$t = \sin \alpha x, \quad t \in [-1, 1]. \tag{19}$$

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

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

we compute

$$\frac{d\psi(x)}{dx} = -\alpha\cos(\alpha x)\frac{dy}{dt}$$
$$\frac{d^2\psi(x)}{dx^2} = \alpha^2\cos^2(\alpha x)\frac{d^2y}{dt^2} - \alpha^2\sin(\alpha x)\frac{dy}{dt}.$$

Then, the equation (17) 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,

$$(1-t^2)\frac{d^2y}{dt^2} - t\frac{dy}{dt} - \frac{u(t)}{\alpha^2}y(t) = \varepsilon y(t), \tag{20}$$

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

Thus, we propose a solution of (20) of the form $y(t) = \sum_{n=0}^{N} y_n \ell_n(t)$, where $\ell_n(t) = \dfrac{T_{N+1}(t)}{(t-t_n)T'_{N+1}(t_n)}$, and t_n, $n = 0,1,\dots,N$ are the zeros of the Chebyshev polynomial $T_{N+1}(t)$ and are known to be

$$t_n = \cos\left(\frac{\pi(n+1/2)}{N+1}\right), \quad n = 0,1,\dots,N. \tag{21}$$

Then we insert this form of $y(t)$ into the equation (20) and require that the equation is satisfied at the nodes t_m for $m = 0,\dots,N$, which gives

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

As a result, we obtain a matrix eigenvalue problem in the form

$$KY = \varepsilon Y, \tag{22}$$

where $K_{mn} = (1-t_m^2)\ell''_n(t_m) - t_m\ell'_n(t_m) - \dfrac{u(t_m)}{\alpha^2}\delta_{mn}$ and $Y = [y_1 \;\; y_2 \;\; \dots y_m]^T$. Using the derivatives of $\ell_n(t_m)$ derived in (15) and (16), and the differential equation of the Chebyshev polynomials we compute the entries of the matrix K as follows.

For $m \neq n$

$$\begin{aligned}
K_{mn} &= (1-t_m^2)\left[\frac{1}{(t_m-t_n)}\frac{T''_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{2}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}\right] - \frac{t_m}{(t_m-t_n)}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} \\
&= \frac{(1-t_m^2)}{(t_m-t_n)}\frac{T''_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} - \frac{t_m}{(t_m-t_n)}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} \\
&= \frac{1}{T'_{N+1}(t_n)}\frac{1}{(t_m-t_n)}\left[(1-t_m^2)T''_{N+1}(t_m) - t_mT'_{N+1}(t_m)\right] - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} \\
&= \frac{1}{T'_{N+1}(t_n)}\frac{1}{(t_m-t_n)}\left[-(N+1)^2T_{N+1}(t_m)\right] - \frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)} \\
&= -\frac{2(1-t_m^2)}{(t_m-t_n)^2}\frac{T'_{N+1}(t_m)}{T'_{N+1}(t_n)}.
\end{aligned}$$

For $m = n$

$$\begin{aligned} K_{nn} &= \frac{(1-t_n^2)}{3}\frac{T'''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{u(t_n)}{\alpha^2} \\ &= t_n\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{u(t_n)}{\alpha^2} \\ &= \frac{t_n}{2}\frac{T''_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2} \\ &= \frac{t_n}{2}\frac{\frac{t_n}{1-t_n^2}T'_{N+1}(t_n) - \frac{(N+1)^2}{(1-t_n^2)}T_{N+1}(t_n)}{T'_{N+1}(t_n)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2} \\ &= \frac{t_n^2}{2(1-t_n^2)} - \frac{N(N+2)}{3} - \frac{u(t_n)}{\alpha^2}. \end{aligned}$$

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

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

6. Legendre pseudospectral formulation

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

$$\left[-\frac{d^2}{dx^2}+v(x)\right]\psi(x)=E\psi(x),\quad x\in(-\infty,\infty). \tag{23}$$

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

$$(1-t^2)P_n''-2tP_n'+n(n+1)P_n=0, \tag{24}$$

we need to apply a transformation on the independent variable x, which transforms the differential operator of the (23) 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

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

With these new variables, (23) is transformed into

$$(1-t^2)\left[(1-t^2)y''(t)-2ty'(t)\right]-\frac{u(t)}{\alpha^2}y(t)=\varepsilon y(t), \tag{25}$$

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

$$y(t)=\sum_{n=0}^{N}y_n\ell_n(t), \tag{26}$$

where

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

and $P_{N+1}(t)$ is the Legendre polynomial of degree $N+1$ and t_n, $n=0,1,\dots,N$ are the zeros of $P_{N+1}(t)$. We put (26) into the equation (25) and require its satisfaction at the nodes $t_0,t_1,\cdots,t_N$. This results in

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

Hence, we obtain a matrix 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 (14), (15) and (16) and the differential equation of Legendre polynomials.

For $m \neq n$

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

For $m = n$

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

In addition, we multiply and divide the off diagonal entries of K_{mn} by $(1-t_n^2)$ which gives

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

where $u(t_n) = v(x_n)$ and $x_n = \frac{1}{2\alpha}\ln\left(\frac{1+t_n}{1-t_n}\right)$. Again, in order to deal with a matrix of simpler 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

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

We have obtained pseudospectral formulations with 2 different types of orthogonal polynomials for the same problem. It should be noticed that, in both 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.

7. Numerical Example

To our knowledge, the Chebyshev and Legendre pseudospectral formulations for the Schrödinger equation with polynomial potential has not been used by other authors before.

The numerical results presented here are given for a polynomial potential

$$v(x) = x^2 + v_4x^4 + v_6x^6 + v_8x^8,$$

with 3 different sets of the coefficients v_4, v_6 and v_8 representing small and large perturbations on the harmonic oscillator. The substitution transforming the infinite interval $(-\infty, \infty)$ to $[-1, 1]$ employed in the previous section contains an optimization parameter $\alpha > 0$. 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 $0.3 < \alpha < 0.4$. For comparison purposes, we used the same values of the coefficients v_4, v_6 and v_8 in both Chebyshev and Legendre pseudospectral methods.

In Tables 1-3, we give the computed eigenvalues of $v(x) = x^2 + v_4x^4$ with $v_4 = 0.1, 1,$ and 5, with both Chebyshev and Legendre pseudospectral methods. Similarly, in Tables 4-6 and Tables 7-9 we present the eigenvalues for $v(x) = x^2 + v_6x^6$ and $v(x) = x^2 + v_8x^8$ with $v_6 = 0.1, 1, 5$ and $v_8 = 0.1, 1, 5$, respectively.

Table 1: Eigenvalues of $v(x) = x^2 + 0.1x^4$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha = 1)$	$E_i^L(\alpha = 1)$	$E_i^C(\alpha = 0.3)$	$E_i^L(\alpha = 0.3)$	$E_i^C(\alpha = 0.4)$	$E_i^L(\alpha = 0.4)$
25	1	0.77821814	1.06523087	1.06528551	1.06528551	1.06528550	1.06528551
	2	2.45684459	3.30572422	3.30687201	3.30687201	3.30687174	3.30687201
	3	5.23643426	5.73925266	5.74795927	5.74795909	5.74795585	5.74795909
	4	10.07118779	8.32476701	8.35267783	8.35267668	8.35264842	8.35267552
	5	17.00870826	11.09039221	11.09859562	11.09860131	11.09840147	11.09859147
35	1	0.77868548	1.06528779	1.06528551	1.06528551	1.06528550	1.06528551
	2	2.45834074	3.30685123	3.30687201	3.30687201	3.30687174	3.30687201
	3	5.23855288	5.74717374	5.74795927	5.74795927	5.74795589	5.74795927
	4	10.07335633	8.34540267	8.35267783	8.35267783	8.35264880	8.35267782
	5	17.01087644	11.06534188	11.09859562	11.09859563	11.09840420	11.09859559

Table 2: Eigenvalues of $v(x) = x^2 + x^4$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha = 1)$	$E_i^L(\alpha = 1)$	$E_i^C(\alpha = 0.3)$	$E_i^L(\alpha = 0.3)$	$E_i^C(\alpha = 0.4)$	$E_i^L(\alpha = 0.4)$
25	1	1.24367760	1.39233946	1.39235165	1.39235128	1.39235164	1.39235164
	2	3.88803404	4.64866785	4.64881273	4.64880867	4.64881270	4.64881250
	3	7.09363103	8.65427283	8.65504716	8.65505802	8.65504996	8.65504682
	4	11.69930683	13.15550075	13.15677362	13.15717124	13.15680390	13.15678589
	5	18.39805834	18.06573383	18.05764381	18.05920876	18.05755743	18.05757240
35	1	1.24430863	1.39235199	1.39235164	1.39235164	1.39235164	1.39235164
	2	3.89138200	4.64881618	4.64881270	4.64881270	4.64881270	4.64881270
	3	7.10071608	8.65505865	8.65504996	8.65504997	8.65504996	8.65504996
	4	11.70835141	13.15669679	13.15680390	13.15680402	13.15680390	13.15680389
	5	18.40737547	18.05630541	18.05755744	18.05755764	18.05755744	18.05755742

Table 3: Eigenvalues of $v(x) = x^2 + 5x^4$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha = 1)$	$E_i^L(\alpha = 1)$	$E_i^C(\alpha = 0.3)$	$E_i^L(\alpha = 0.3)$	$E_i^C(\alpha = 0.4)$	$E_i^L(\alpha = 0.4)$
25	1	2.00513163	2.01833959	2.01833601	2.01828991	2.01834063	2.01834071
	2	6.90747928	7.01346291	7.01316949	7.01291597	7.01347884	7.01348552
	3	12.98420734	13.46760044	13.46519639	13.46822754	13.46772812	13.46781824
	4	19.39380318	20.81342486	20.81942817	20.84355093	20.81397885	20.81423059
	5	26.18319353	28.87454546	29.00067237	28.92968083	28.87523713	28.87251179
35	1	2.00524431	2.01834064	2.01834065	2.01834069	2.01834065	2.0183406
	2	6.90848786	7.01347917	7.01347917	7.01347971	7.01347919	7.01347919
	3	12.98942369	13.46773091	13.46773099	13.46773250	13.46773041	13.46773042
	4	19.41042879	20.81397517	20.81397358	20.81393729	20.81396694	20.81396676
	5	26.21584221	28.87505117	28.87499743	28.87466289	28.87499635	28.87499442

Table 4: Eigenvalues of $v(x) = x^2 + 0.1x^6$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
25	1	0.82136037	1.10913158	1.10908704	1.10908493	1.10908708	1.10908741
	2	2.59735307	3.59673752	3.59603643	3.59600962	3.59603692	3.59603941
	3	5.42573191	6.64912266	6.44438870	6.64423837	6.64439171	6.64439256
	4	10.23766105	10.25553004	10.23786735	10.23755840	10.23787372	10.23776622
	5	17.14686086	14.33495987	14.30710440	14.30905999	14.30704008	14.30612198
35	1	0.82213901	1.10907701	1.10908708	1.10908708	1.10908708	1.10908708
	2	2.59998114	3.59592271	3.59603692	3.59603697	3.59603692	3.59603692
	3	5.42963941	6.64373424	6.64439171	6.64439222	6.64439171	6.64439168
	4	10.24177732	10.23548559	10.23787372	10.23787711	10.23787372	10.23787326
	5	17.15099475	14.30209050	14.30704004	14.30705410	14.30704005	14.30703642

Table 5: Eigenvalues of $v(x) = x^2 + x^6$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
25	1	1.34804349	1.43562558	1.43562823	1.43558113	1.43562447	1.43561421
	2	4.53988151	5.03347855	5.03325961	5.03247659	5.0339510	5.03333064
	3	8.58481692	9.96748576	9.94661527	9.95858376	9.96662356	9.96653816
	4	13.57703878	15.99435165	15.97578910	15.95052610	15.98948891	15.99069217
	5	20.12211425	22.92784888	22.86784451	22.84082832	22.91056041	22.92124380
35	1	1.34888050	1.43562563	1.43562469	1.43562568	1.43562462	1.43562466
	2	4.54486603	5.03340355	5.0339666	5.03340564	5.03339594	5.03339632
	3	8.59888479	9.96665256	9.96662637	9.96667250	9.96662200	9.96662421
	4	13.60123088	15.98949774	15.98945494	15.98955950	15.98944078	15.98944883
	5	20.15213249	22.90999893	22.91016767	22.90978486	22.91018039	22.91018978

Table 6: Eigenvalues of $v(x) = x^2 + 5x^6$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
25	1	1.90917691	1.91245513	1.91128342	1.91085538	1.91243877	1.91238806
	2	6.93892856	6.96089620	6.95341081	6.95314702	6.96078634	6.96070105
	3	14.07706707	14.16947735	14.16134290	14.18357771	14.16930401	14.17155146
	4	22.73502342	23.04369447	23.19954684	23.31496132	23.04540916	23.06414338
	5	32.42847415	33.28107701	34.07590753	34.26916982	33.29729901	33.37039412
35	1	1.90923202	1.91245379	1.91246042	1.91248042	1.91245381	1.91245304
	2	6.93931952	6.96085722	6.96092740	6.96109653	6.96085699	6.96085129
	3	14.07885754	14.16910270	14.16958004	14.17040873	14.16909876	14.16907771
	4	22.74167405	23.04155561	23.04331861	23.04489094	23.04152663	23.04151125
	5	32.44902932	33.27303422	33.27378287	33.26561440	33.27289621	33.27331610

Table 7: Eigenvalues of $v(x) = x^2 + 0.1x^8$ with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
$N=25$	1	0.90040430	1.16881854	1.16899756	1.16913690	1.16897047	1.16894127
	2	2.86499847	3.93821953	3.93990939	3.94098877	3.93972209	3.93945483
	3	5.81131004	7.63178440	7.64054004	7.64485274	7.63995660	7.63859306
	4	10.60557592	12.24915931	12.28114575	12.28950933	12.28121949	12.27622222
	5	17.46496405	17.66611997	17.74989850	17.73603399	17.76146648	17.74875867
$N=35$	1	0.901189675	1.16896057	1.16897056	1.16897315	1.16897045	1.16897080
	2	2.87053538	3.93966773	3.93972209	3.93974585	3.93972136	3.93972436
	3	5.82033292	7.63985744	7.63995081	7.64007691	7.63994849	7.63996323
	4	10.61569369	12.28152126	12.28116835	12.28164349	12.28116774	12.28122019
	5	17.47530759	17.76457982	17.76117289	17.76247695	17.76121363	17.76135008

Table 8: Eigenvalues of $v(x) = x^2 + x^8$ with with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
$N=25$	1	1.45443154	1.49097356	1.49164297	1.49216006	1.49097978	1.49086529
	2	5.16194558	5.36831059	5.37097110	5.37213067	5.36846606	5.36724388
	3	10.33082783	10.99095419	10.98828972	10.97822409	10.99224891	10.98468049
	4	16.63046206	18.17871483	18.09571790	18.00542654	18.18568101	18.15180974
	5	23.91095664	26.70030474	26.27554829	25.93402071	26.73006112	26.62129447
$N=35$	1	1.45510986	1.49101798	1.49100936	1.49096002	1.49097978	1.49101644
	2	5.16602825	5.36876016	5.36873050	5.36845373	5.36877730	5.36874817
	3	10.34482556	10.99363375	10.99374600	10.99308585	10.99373476	10.99357409
	4	16.66484594	18.19062967	18.19210062	18.19227448	18.19109499	18.19039319
	5	23.97352728	26.74169159	26.75085878	26.76228292	26.74345735	26.74099783

Table 9: Eigenvalues of $v(x) = x^2 + 5x^8$ with with with Chebyshev E_i^C and Legendre E_i^L pseudospectral methods for $\alpha = 1; 0.3$ and 0.4.

N	i	$E_i^C(\alpha=1)$	$E_i^L(\alpha=1)$	$E_i^C(\alpha=0.3)$	$E_i^L(\alpha=0.3)$	$E_i^C(\alpha=0.4)$	$E_i^L(\alpha=0.4)$
$N=25$	1	1.88703727	1.88737455	1.88160102	1.88052064	1.88719192	1.88631521
	2	7.00825824	7.01018966	6.98460727	6.98416575	7.00966632	7.00541507
	3	14.66930090	14.67622047	14.67627429	14.70828891	14.67948901	14.67272087
	4	24.51315063	24.53428274	24.88139816	25.04460675	24.56795683	24.58737554
	5	36.20185978	36.26315566	38.12924093	38.93640760	36.44855707	36.64593094
$N=35$	1	1.88704900	1.88748848	1.88770418	1.88791810	1.88748206	1.88746088
	2	7.00833002	7.01093701	7.01255689	7.01413864	7.01089533	7.01071889
	3	14.66958128	14.67928516	14.68746710	14.69506790	14.67911762	14.67816555
	4	24.51407592	24.54405987	24.57308431	24.59775636	24.54354400	24.53947908
	5	36.20462164	36.28693355	36.35470965	36.40150930	36.28593542	36.27237435

8. Conclusion

The Schrödinger equation for anharmonic oscillator studied in this paper is a originally defined on the infitine interval $(-\infty, \infty)$. Therefore, it is natural to propose a pseudospectral method based on Hermite polynomials. Also, one can use a substitution which transforms the interval to $(0, \infty)$ and propose pseudospectral scheme based on Laguerre polynomials. On the other hand, the numerical calculations presented in the previous section show that the problem can be also treated via pseudospectral methods based on Chebyshev and Legendre polynomials. This approach provides a different aspect for the use pseudospectral methods with Chebyshev and Legendre polynomials which are usually not considered very often since most of the one dimensional Schrödinger equations are defined on infinite intervals.

Numerical results also show the benefit of using an optimization parameter which improves the accuracy with smaler size matrices. However, the choice of an optimal value for this parameter is not theoretically verified and one should determine this optimal value only experimentally.

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