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Numerical Solution of Linear Ordinary Differential Equations in Quantum Chemistry by Clenshaw Method

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***Abstract*—**As we know, most differential equations concerning physical phenomenon could not be solved by analytical method. Even if we use Series Method, some times we need an appropriate change of variable, and even when we can, their closed form solution may be so complicated that using it to obtain an image or to examine the structure of the system is impossible. For example, if we consider Schrodinger equation, i.e.,

$$\varphi'' + (2mE^{-2} - \alpha^2 x^2)\varphi = 0,$$

We come to a three-term recursion relations, which work with it takes, at least, a little bit time to get a series solution[6]. For this reason we use a change of variable such as

$$\varphi = e^{-\alpha x^2/2} f(x),$$

or when we consider the orbital angular momentum[1], it will be necessary to solve

$$\frac{d^2 s}{d\theta^2} + \cot\frac{ds}{d\theta} + \left(\frac{c}{h^2} - \frac{m^2}{\sin^2\theta}\right)s = 0.$$

As we can observe, working with this equation is tedious.

In this paper, after introducing Clenshaw method, which is a kind of Spectral method, we try to solve some of such equations.

***Keywords*—**Chebyshev polynomials, Clenshaw method, ODEs, Spectral methods.

I. INTRODUCTION

THE spectral methods arises from the fundamental problem of approximation of a function by interpolation on an interval, and are very much successful for the numerical solution of ordinary or partial differential equations[1]. Since the time of Fourier(1882), spectral representations in analytic study of differential equations are used and their applications for numerical solution of ordinary differential equations refers, at least, to the time of Lanczos[2]. Spectral methods have become increasingly popular, especially, since the development of Fast transform methods, with applications in numerical weather predication, numerical Simulations of turbulent flows, and other problems where high accuracy is desired for complicated solutions.

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A survey of some application is given in [3]. Spectral methods may be viewed as an extreme development of the class of discretization scheme for differential equations known generally as the method of weighted residuals (MVR) (Finlayson and Scriren (1966)). The key elements of the MWR are the trial functions (also called approximating functions) which are used as basis functions for a truncated series expansion of the solution, and the test functions (also known as weight functions) which are used to ensure that the differential equation is satisfied as closely as possible by the truncated series expansion. The choice of such functions distinguishes between the three most commonly used spectral schemes, namely, Galerkin, collocation (also called pseudo-spectral) and Tau version. The Tau approach is a modification of Galerkin method that is applicable to problems with non-periodic boundary conditions. In broad terms, Galerkin and Tau methods are implemented in terms of the expansion coefficients, where as collocation methods are implemented in terms of physical space values of unknown function. The basic of spectral methods to solve differential equations is to expand the solution function as a finite series of very smooth basis function, as given

$$y^N(x) = \sum_{k=0}^{N} a_k \phi_k(x), \qquad (1)$$

in which, as we know, the best choice of ϕ_k, are the eigenfunctions of a singular Sturm-Liouville problem. If the function y belongs to $C^\infty[a,b]$, the produced error of approximation (1), when N tends to infinitly, approaches zero with exponential rate [1]. This phenomenon is usually referred to as "spectral accuracy", [3]. The accuracy of derivatives obtained by direct, term by term differentiation of such truncated expansion naturally deteriorates [1], but for low order derivatives and sufficiently high-order truncations this deterioration is negligible .So, if solution function and coefficient functions are analytic on $[a,b]$, spectral methods will be very efficient and suitable.

II. SPECTRAL METHODS

In this section, we are going, briefly, to introduce spectral methods. For this reason, first we consider the following differential equation :

$$Ly = \sum_{i=0}^{M} f_{M-i}(x) D^i y = f(x) \;, \; x \in [-1,1] \;, \qquad (2)$$

$$Ty = C \;, \qquad (3)$$

Where f_i , $i = 0,1,...,M$, f ,are known real functions of x, D^i denotes i^{th} order of differentiation with respect to x, T is a linear functional of rank N and $C \in \Re^M$.

Here (3) can be initial, boundary or mixed conditions. The basic of spectral methods to solve this class of equations is to expand the solution function, y , in (2) and (3) as a finite series of very smooth basis function, as given below

$$y^N(x) = \sum_{k=0}^{N} a_k T_k(x) \qquad (4)$$

Where, $\{T_k(x)\}_0^k$ is sequence of Chebyshev polynomials of first kind, defined as, $T_n(x) = \cos(n \cos^{-1} x)$, $n = 0,1,...$

With replacing y^N in (2), we define residual term by $r^N(x)$ as follows

$$r^N(x) = Ly^N - f \;. \qquad (5)$$

In spectral methods, main target is to minimize $r^N(x)$, through domain as much as possible with regard to(3). Implementatian of these methods lead to a system of linear equations with $N+1$ equations and $N+1$ unknowns $a_0, a_1, ..., a_N$.

In rest of this section, we discuss, briefly, three spectral methods, namely, Tau, Galerkin and collocation (also known as pseudo- and use it for numerical solution of second order linear differential equations. It is to be noted that this discussion can be extended to the general form (2),(3).

A. Tau method

Consider the following linear ordinary differential equation(ODE) :

$$P(x)\, y'' + Q(x)\, y' + R(x)\, y = S(x) \;, x \in (-1,1) \;,$$
$$y(-1) = \alpha \;, \; y(1) = \beta \;.$$

Our target is to find, $\underline{a} = (a_0, a_1, ..., a_N)^t$. For this reason, we multiply both sides of (1) by

$$\frac{2}{\pi\, c_j} \int_{-1}^{1} \frac{T_j(x)}{\sqrt{1-x^2}}\, dx \;, \; j = 0,1,2,..., \; N-2,$$

to obtain

$$\frac{2}{\pi\, c_j} \sum_{i=0}^{N} a_i \int_{-1}^{1} \frac{\phi_i(x) T_j(x)}{\sqrt{1-x^2}}\, dx = \frac{2}{\pi\, c_j} \int_{-1}^{1} \frac{S(x) T_j(x)}{\sqrt{1-x^2}}\, dx.$$

Here, to compute the right-hand side of this equation it is sufficient to use an appropriate numerical integration method such as Gauss-Chebyshev method.

B. Galerkian method

This method is similar to tau method, where $N-1$ basis functions $\psi_2, \psi_3, ..., \psi_N$, are obtained through Chebyshevpolynomials $T_0, T_1, ..., T_N$, in order to satisfy both boundary conditions (6). Then we multiply both sides of (1) by

$$\int_{-1}^{1} \frac{\psi_j(x)}{\sqrt{1-x^2}}\, dx \;, \quad j = 2, 3, \ldots, N \;,$$

to obtain $N-1$ equations.

C. Pseudo-spectral method

In this method, we substitute points $x_j = \cos(\frac{\pi j}{N}),\; j = 1,2,..., N-1,$ in (1) and put:

$$y^N(x_j) = \sum_{i=0}^{N} a_i \phi_i(x_j), \;\; j = 1,2,..., \; N-1,$$

to obtain N-1 equations.

Now we are going to introduce Clenshaw method and use it for numerical solution of linear(ODEs).

III. CLENSHAW METHOD

Consider the following linear ODE:

$$P(x)\, y'' + Q(x)\, y' + R(x)\, y = S(x) \;, x \in (-1,1) \;,$$
$$y(-1) = \alpha \;, \; y(1) = \beta \;. \qquad (6)$$

First, for an arbitrary natural number, N , we suppose that the approximate solution of equations (6) is given by (4). Our target is to find $\underline{a} = (a_0, a_1, ..., a_N)^t$ .For this reason, put

$$P(x) \approx \sum_{i=0}^{N} \xi_i T_i(x),$$

$$Q(x) \approx \sum_{i=0}^{N} \gamma_i T_i(x), \qquad (7)$$

$$R(x) \approx \sum_{i=0}^{N} \lambda_i T_i(x).$$

Using this fact that the Chebyshev expansion of a function

$u \in L_w^2(-1,1)$ is

$$u(x)=\sum_{k=0}^{\infty}\hat{u}_k T_k(x)\ ;\ \hat{u}_k=\frac{2}{\pi c_k}\int_{-1}^{1}u(x)T_k(x)\,w(x)\,dx,$$

we can find coefficients ξ_i, λ_i and λ_i as follows :

$$\xi_i=\frac{2}{\pi c_i}\int_{-1}^{1}\frac{P(x)T_i(x)}{\sqrt{1-x^2}}dx$$
$$\gamma_i=\frac{2}{\pi c_i}\int_{-1}^{1}\frac{Q(x)T_i(x)}{\sqrt{1-x^2}}dx \qquad (8)$$
$$\lambda_i=\frac{2}{\pi c_i}\int_{-1}^{1}\frac{R(x)T_i(x)}{\sqrt{1-x^2}}dx,$$

where, $c_0=2$ and $c_i=1$, for $i\geq 1$.

To compute the right-hand side of (8) it is sufficient to use an appropriate numerical integration method. Here, we use $(N+1)$ points Chebyshev-Gauss-Lobatto quadrature given as;

$$x_j=\cos\frac{\pi j}{N},\ w_j=\frac{\pi}{\tilde{c}_j N},\ 0\leq j\leq N\ ,$$

where, $\tilde{c}_0=\tilde{c}_N=2$ and $\tilde{c}_j=1$ for $j=1,2,...,N-1$. Note that for simplicity of the notation these points are arranged in descending order, namely $,x_N<x_{N-1}<...<x_1<x_0$.

with weights

$$w_k=\frac{\pi}{N}\ ,\quad 1\leq k\leq N-1\ ,$$
$$=\frac{\pi}{2N}\ ,\quad k=0\ ,k=N\ ,$$

and node points $x_k=\cos\frac{\pi k}{N}$, $k=0,1,...,N$. That is, we put, [4]:

$$\xi_i\approx\frac{\pi}{N}\sum_{k=0}^{N}{}'' P(\cos(\frac{k\pi}{N}))\,T_i(\cos(\frac{k\pi}{N}))\ ,$$

and using $T_i(x)=\cos(i\cos^{-1}x)$, we get

$$\xi_i\approx\frac{\pi}{N}\sum_{k=0}^{N}{}'' P(\cos(\frac{k\pi}{N}))\,\cos(\frac{\pi ik}{N})\ ,$$

Where, notation $\sum''$ means first and last terms become half .Therefore, we will have :

$$\xi_i\approx\frac{\pi}{N}\sum_{k=0}^{N}{}'' P(\cos(\frac{k\pi}{N}))\,\cos(\frac{\pi ik}{N})\ ,$$
$$\gamma_i\approx\frac{\pi}{N}\sum_{k=0}^{N}{}'' Q(\cos(\frac{k\pi}{N}))\cos(\frac{\pi ik}{N}), \qquad (9)$$
$$\lambda_i\approx\frac{\pi}{N}\sum_{k=0}^{N}{}'' R(\cos(\frac{k\pi}{N}))\,\cos(\frac{\pi ik}{N})\ .$$

Now, replacing (4) and (9) in equations (6), and using this fact that

$$y'(x)\approx\sum_{m=0}^{N}a_m^{(1)}T_m(x)\ ,\ a_m^{(1)}=\frac{2}{c_m}\sum_{\substack{p=m+1\\ m+p=odd}}^{N}pa_p\ ,\ m=0,1,...,N-1\ ,$$

$$y''(x)\approx\sum a_m^{(2)}T_m(x),\ a_m^{(2)}=\frac{2}{c_m}\sum_{\substack{p=m+2\\ m+p=even}}^{N}p(p^2-m^2)a_p\ ,m=0,1,...,N-2,\ a_{N-1}^{(2)}=a_N^{(2)}=0$$

In this manner, we get

$$\sum_{i=0}^{N}\sum_{m=0}^{N}\lambda_i a_m^{(2)}T_i(x)T_m(x)+\sum_{i=0}^{N}\sum_{m=0}^{N}\gamma_i a_m^{(1)}T_i(x)T_m(x)+$$
$$\sum_{i=0}^{N}\sum_{m=0}^{N}\xi_i a_m T_i(x)T_m(x)=S(x)\ , \qquad (10)$$

$$\sum_{i=0}^{N}a_iT_i(-1)=\alpha\ ,$$
$$\sum_{i=0}^{N}a_iT_i(1)=\beta\ . \qquad (11)$$

Now, we multiply both sides of (10) by $\frac{2}{\pi c_j}\frac{T_j(x)}{\sqrt{1-x^2}}$, and integrating from -1 to 1, gives

$$\frac{2}{\pi c_j}\sum_{i=0}^{N}\sum_{m=0}^{N}[\lambda_i a_m^{(2)}+\gamma_i a_m^{(1)}+\xi_i a_m]\int_{-1}^{1}\frac{T_i(x)T_m(x)T_j(x)}{\sqrt{1-x^2}}dx$$

$$=\frac{2}{\pi c_j}\int_{-1}^{1}\frac{S(x)T_j(x)}{\sqrt{1-x^2}}dx,\ j=0,1,...N-2, \qquad (12)$$

where,

$$\int_{-1}^{1}\frac{T_i(x)T_m(x)T_j(x)}{\sqrt{1-x^2}}dx = \begin{cases}\pi & ,i=m=j=0,\\ \frac{\pi}{2}\delta_{i,m} & ,i+m>0,\, j>0,\\ \frac{\pi}{4}(\delta_{j,i+m}+\delta_{j,|i-m|}), & j>0\end{cases} \quad (13)$$

with, $\delta_{i,j}=1$,when $i=j$,and zero when $i\neq j$,[5] .

We also can use $N+1$ points Chebyshev-Gauss-Lobatto quadrature to compute right-hand side integration .Therefore, with replacing (13) in (12) and using this fact that $T_i(\pm 1)=(\pm 1)^i$, equations (12) and (11) make a system of $N+1$ equations and $N+1$ unknown $a_0, a_1, ..., a_N$, we can obtain from this system $(a_0, a_1, ..., a_N)^t$ to obtain $N-1$ equations.

IV.NUMERICAL EXAMPLES

Here we consider some ordinary differential equations problems with Clenshaw method and discuss the results.

We start this section with Schrodinger equation.

Example 1: Let us consider

$$\varphi'' + (2mEh^{-2} - \alpha^2 x^2)\varphi = 0.$$

Let's $\alpha = 2,\ mEh^{-2} = -1,$ with y(0)=1, y(1)=e and exact solution $y(x)=e^{x^2}$. Using change of variable such as $t=(x+1)/2$ we can transfer interval [0,1] to [-1,1].

We solved this equation by Clenshaw method and compare the results with different values of N. The results for $N=4,7,10,13,$ respectively, were;

$$1.660\times10^{-2}, 4.469\times10^{-5}, 5.901\times10^{-8}, 7.730\times10^{-11}.$$

As we expected when N increases errors decrease.

Example.2: Consider Legendre's equation,

$$(1-x^2)y'' - 2xy' + \lambda(\lambda+1)y = 0.$$

As we know, this equation for $\lambda = 1,$ and boundary conditions $y(\pm 1) = -2,$ has solution $y(x) = 1-3x^2.$

We choose $N = 4,\ 6,10$ and the results were;

$$5.5511\times10^{-17}, 2.2204\times10^{-16}, 2.7756\times10^{-17}.$$

Since our solution is a polynomial then for $N \geq 3,$ we come to a solution with error zero. If you find the error is not zero but close to it, is because of rounding error. We must put in our mind this method is so good whenever the exact solution is a polynomial.

Example 3: Let's consider Laguerre's equation given by;

$$xy'' + (1-x)y' + \lambda y = 0.$$

Suppose $\lambda = 2,$ with boundary conditions $y(-1) = 7/2, y(1) = -1/2.$

The exact solution is $y(x) = 1-2x+x^2/2$. Here we have, again a polynomial solution so we expect solutions with very small error. We examined for different values of N such as $N = 2,3$ and get the results 0, 2.7756×10^{-17}.

A nice discussion was published whenever coefficient functions or solution function are not analytic [7].

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