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ON THE NUMERICAL SOLUTION OF ONE DIMENSIONAL SCHRODINGER EQUATION WITH BOUNDARY CONDITIONS INVOLVING FRACTIONAL DIFFERENTIAL OPERATORS

B. Jazbi & M. Moini

Abstract: *In this paper we study of collocation method with Radial Basis Function to solve one dimensional time dependent Schrodinger equation in an unbounded domain. To this end, we introduce artificial boundaries and reduce the original problem to an initial boundary value problem in a bounded domain with transparent boundary conditions that involves half order fractional derivative in t. Then in three stages we use the Laplace Transform method, the collocation method and finally the Legender expansion method. Numerical examples are given to show the effectiveness of the scheme.*

Keywords: *The Schrodinger equation, Collocation method, Radial Basis Function, Fractional derivative boundary condition, Legendre expansion method*

1. Introduction

The time dependent Schrodinger equation is the base of quantum mechanics [1, 2]. This model equation also arises in many other practical domains of physical and technological interest, e.g. optics, seismology and plasma physics. There are a lot of studies on the numerical solution of initial-boundary problems for solving the linear or nonlinear Schrodinger equation [3, 4, 5, 6]. When we want to solve numerically a differential equation defined on an infinite domain, it is necessary to consider a finite sub domain and to use artificial boundary conditions in such a way that the solutions in the finite sub domain approximate the original solution. If the approximation is exact, the transfer is called exact and the corresponding artificial boundary condition is called exact or transparent.

In this paper application of the collocation method with RBF to solve one dimensional time dependent Schrodinger equation is investigated.

A fairly new approach to solving PDEs is through Radial Basis Functions (RBFs). The RBFs depend only on the distance say $\psi(\| x - x_i \|)$, where $\|.\|$ denotes the Euclidean norm. The RBFs may also have a shape parameter c, in which case $\psi(r)$ is replaced with $\psi(r,c)$, where $\psi(r)$ is some function defined for $r \geq 0$. The most popular RBFs are given as follows:

(1) Multiquadrics (MQ):

$$\psi(r) = (r^2 + c^2)^{\frac{\beta}{2}}, \ \beta = 1,3,5,...,2N+1,...,$$

(2) Inverse Multiquadrics (IMQ):

$$\psi(r) = (r^2 + c^2)^{\frac{\beta}{2}}, -\beta = 1, 3, 5,..., 2N+1,...,$$

(3) Gaussians (GA):

$$\psi(r) = \exp(-c^2 r^2),$$

(4) Inverse quadrics (IQ):

$$\psi(r) = (r^2 + c^2)^{-1}.$$

A key feature of an RBF method is that it does not require a grid. The only geometric properties that are used in an RBF approximation are the pair-wise distances between points. Since the distances are easy to compute therefore working in higher dimensions spatial space does not increase the computational time. The method works with points scattered throughout the domain of interest, and the RBF interpolant is a linear combination of RBFs centered at the scattered points x_i:

$$s(x,c) = \sum_{i=1}^{n} \lambda_i \, \psi\left(\left\| x - x_i \right\|, c\right),$$

where the coefficients λ_i are usually determined by collocation with given discrete data, such as function values or derivative information. For study more about this discussion see the book by Cheney and Light [7].

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B. Jazbi is with the Department of Mathematics, Iran University of Science and Technology, Tehran, Iran. *E-mail*: jazbi @iust.ac.ir
M. Moini is with the Department of Mathematics, Iran University of Science and Technology, Tehran, Iran, *E-mail*: m-moini@iust.ac.ir.

The remainder of this paper is organized as follows: in section 2 we introduce one dimensional time dependent Schrodinger equation with transparent boundary conditions (TBCs) and the construction of the discrete scheme. In section 3 we give collocation method with RBFs for approximation the problem. The inversion formula for the Laplace transform is described in section 4. The numerical results are proposed in section 5.

2. The Construction of the Discrete Scheme

In this paper, we consider the following linear equation [8]:

$$i\frac{\partial u}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + V(x,t)u(x,t) \quad , \quad \forall (x,t) \in \Omega , \qquad (1)$$

$$u(x,0) = u^0(x) \quad , \qquad -\infty < x < +\infty \quad ,$$

Where $\Omega = \{(x,t) \mid -\infty < x < +\infty, 0 < t \le T\}$, $V(x,t)$ designates a given potential (real valued) function on Ω, $u^0(x)$ is the complex initial data given on R, and the unknown function $u(x,t)$ is a complex value function on Ω. Let us split the initial domain Ω into three regions. For this reason, first we introduce two artificial boundaries as follows:

$$\Pi_0 = \{(x,t) \mid x = 0,\ 0 < t \le T\},$$
$$\Pi_1 = \{(x,t) \mid x = 1,\ 0 < t \le T\}.$$

Then the domain Ω is divided into three parts. Two unbounded parts are as follows:

$$\Omega_0 = \{(x,t) \mid -\infty < x \le 0,\ 0 < t \le T\},$$
$$\Omega_1 = \{(x,t) \mid 1 \le x < +\infty,\ 0 < t \le T\},$$

and one bounded part is:

$$\Omega^c = \{(x,t) \mid 0 < x < 1,\ 0 < t \le T\}.$$

The finite sub domain Ω^c is our computational domain. Let $V(x,t) = 1$ and u^0 is compact support with:

$$\sup p\{u^0\} \subset [0,1].$$

We consider the restriction of the solution of problem (1) on the domain Ω^c. The TBCs for Schrodinger equation have been independently derived by several authors from various application fields [9, 10]. They are non-local in t and read:

$$\frac{\partial u}{\partial x}(0,t) = \sqrt{\frac{2}{\pi}}\, e^{-i\frac{\pi}{4}-it}\, \frac{d}{dt}\int_0^t \frac{u(0,\mu)e^{i\mu}}{\sqrt{t-\mu}}d\mu \quad , on \ \Pi_0 , \qquad (2)$$

$$\frac{\partial u}{\partial x}(1,t) = -\sqrt{\frac{2}{\pi}}\, e^{-i\frac{\pi}{4}-it}\, \frac{d}{dt}\int_0^t \frac{u(1,\mu)e^{i\mu}}{\sqrt{t-\mu}}d\mu \quad , on \ \Pi_1 . \qquad (3)$$

Using the notations of the Riemann- Liouville fractional derivative, the boundary conditions (2) and (3) can be written as:

$$\frac{\partial u}{\partial x}(0,t) = \sqrt{2}\, e^{-i\frac{\pi}{4}-it}\, \frac{d^{\frac{1}{2}}[u(0,t)e^{it}]}{dt^{\frac{1}{2}}} , \ on \ \Pi_0 ,$$

$$\frac{\partial u}{\partial x}(1,t) = -\sqrt{2}\, e^{-i\frac{\pi}{4}-it}\, \frac{d^{\frac{1}{2}}[u(1,t)e^{it}]}{dt^{\frac{1}{2}}} , \ on \ \Pi_1 .$$

As a consequence, the boundary value problem to approximate is now given by:

$$i\frac{\partial u}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + u(x,t) \quad , \quad \forall (x,t) \in \Omega^c , \qquad (4)$$

$$\frac{\partial u}{\partial x}(0,t) = \sqrt{\frac{2}{\pi}}\, e^{-i\frac{\pi}{4}-it}\, \frac{d}{dt}\int_0^t \frac{u(0,\mu)e^{i\mu}}{\sqrt{t-\mu}}d\mu , \quad 0 < t \le T \quad , \qquad (5)$$

$$\frac{\partial u}{\partial x}(1,t) = -\sqrt{\frac{2}{\pi}}\, e^{-i\frac{\pi}{4}-it}\, \frac{d}{dt}\int_0^t \frac{u(1,\mu)e^{i\mu}}{\sqrt{t-\mu}}d\mu , \quad 0 < t \le T , \qquad (6)$$

$$u(x,0) = u^0(x) \quad , \qquad 0 \le x \le 1 \quad .$$

This initial boundary value problem is well-posed and its solution coincides with the solution of the original problem (1) restricted to $\overline{\Omega}^c$ [11].
Here, we focus on discrete model for boundaries. We consider $u(0,0) = u(1,0) = 0$ and let:

$$\frac{d}{dt}\int_0^t \frac{u(0,\mu)e^{i\mu}}{\sqrt{t-\mu}}d\mu = 2\frac{d}{dt}\int_0^t \sqrt{t-\mu}\,\frac{d}{d\mu}\{u(0,\mu)e^{i\mu}\}d\mu = \int_0^t \frac{d}{d\mu}(u(0,\mu)e^{i\mu})\frac{d\mu}{\sqrt{t-\mu}} . \qquad (7)$$

According to the equation (7), we can rewrite equations (5) and (6) as follows:

$$\frac{\partial u}{\partial x}(0,t)=\sqrt{\frac{2}{\pi}}e^{-i\frac{\pi}{4}-it}\int_0^t\frac{d}{d\mu}(u(0,\mu)e^{i\mu})\frac{d\mu}{\sqrt{t-\mu}}\ , \qquad (8)$$

$$\frac{\partial u}{\partial x}(1,t)=-\sqrt{\frac{2}{\pi}}e^{-i\frac{\pi}{4}-it}\int_0^t\frac{d}{d\mu}(u(1,\mu)e^{i\mu})\frac{d\mu}{\sqrt{t-\mu}}\ . \qquad (9)$$

By applying Laplace transform for equations (4), (8) and (9), we have:

$$i(sU(x,s)-u(x,0))=-\frac{1}{2}\frac{\partial^2 U}{\partial x^2}(x,s)+U(x,s)\ ,$$
$$\forall(x,s)\in\Omega^e\ , \qquad (10)$$

$$\frac{\partial U}{\partial x}(0,s)=Ks\sqrt{\frac{\pi}{s+i}}U(0,s)\ ,\ \delta_0<s<\infty\ , \qquad (11)$$

$$\frac{\partial U}{\partial x}(1,s)=-Ks\sqrt{\frac{\pi}{s+i}}U(1,s)\ ,\ \delta_0<s<\infty\ , \qquad (12)$$

where:

$$K=\sqrt{\frac{2}{\pi}}e^{-i\frac{\pi}{4}}\qquad ,\qquad U(x,s)=L(u(x,t))\ ,$$

$$\Omega^e=\left\{(x,s)\,\middle|\,0<x<1\ ,\ \delta_0<s<\infty\right\}.$$

For discretization, we consider:

$$h=\frac{1}{N}\ ,$$

where N is positive integer and h is spatial sizes. The one dimensional nodal points are defined as:

$$x_i=ih\quad ,\quad i=0,1,2,...,N\ .$$

3. Description of the Collocation Method With RBF

In this section, we study collocation method with RBF. Let $\{x_i\}_{i=0}^N$ be $N+1$ distinct collocation nodal points in $[0,1]$. In this study we consider multiquadric RBFs as defined as:

$$\psi_i(x)=\psi(r_i)=\sqrt{r_i^2+c}\ ,\ c>0\ ,\ i=0,1,2,...,N\ ,$$

where:

$$r_i=\|x-x_i\|\ .$$

The unknown function $u(x,t)$ can be approximated as:

$$u(x,t)=\sum_{i=0}^{N}a_i(t)\psi_i(x)\ , \qquad (13)$$

and it's Laplace transform:

$$U(x,s)=\sum_{i=0}^{N}\hat{a}_i(s)\psi_i(x)\ , \qquad (14)$$

where :

$$\hat{a}_i(s)=L(a_i(t))\quad ,$$

and $\hat{a}_i(s)$ is unknown and $\psi_i(x)$ is known. By using collocation method for PDE, we have the following equation:

$$res(x_k,s)=0\quad ,\qquad k=1,2,...,N-1\ . \qquad (15)$$

Substituting (13) and (14) into (15), we can obtain the following scheme:

$$is\sum_{i=0}^{N}\hat{a}_i(s)\psi_i(x_k)-i\sum_{i=0}^{N}a_i(0)\psi_i(x_k)=$$
$$-\frac{1}{2}\sum_{i=0}^{N}\hat{a}_i(s)\psi_i^{''}(x_k)+\sum_{i=0}^{N}\hat{a}_i(s)\psi_i(x_k)\ .$$

After simplify, we have:

$$D_{k0}(s)\hat{a}_0(s)+...+D_{kN}(s)\hat{a}_N(s)=$$
$$B_{k0}a_0(0)+...+B_{kN}a_N(0)\quad , \qquad (16)$$

Where:

$$D_{kj}(s)=(s-\frac{1}{i})B_{kj}+\frac{1}{2}p_{kj}\ ,$$
$$B_{kj}=i[(k-j)^2h^2+c]^{\frac{1}{2}}\ ,$$
$$p_{kj}=\frac{1}{\sqrt{[(k-j)^2h^2+c]}}-\frac{(k-j)^2h^2}{\sqrt{[(k-j)^2h^2+c]^3}}\ ,$$
$$k=1,\ 2,...,\ N-1\ ,\ j=0,1,...,\ N\ .$$

Therefore, substituting (14) into (11) and (12), we can obtain the following scheme:

$$Ks\eta\ \hat{a}_0(s)+W_1\hat{a}_1(s)+...+W_N\hat{a}_N(s)=0\ , \qquad (17)$$

$$Q_N\hat{a}_0(s)+...+Q_1\hat{a}_{N-1}(s)+Ks\eta\ \hat{a}_N(s)=0, \qquad (18)$$

Where:

$$W_j(s) = Ks\sqrt{\frac{\pi}{s+i}}\ \gamma_j + \lambda_j \ ,\ j = 0,1,...,\ N \ ,$$

$$Q_j(s) = Ks\sqrt{\frac{\pi}{s+i}}\ \gamma_j - \lambda_j \ \ ,$$

$$\gamma_j = \sqrt{(jh)^2 + c} \qquad ,$$

$$\lambda_j = \frac{jh}{\gamma_j} , \qquad \eta = \sqrt{\frac{c\pi}{s+i}} \ .$$

Introducing the state vector :

$$\hat{a}(s) = (\hat{a}_0(s), \hat{a}_1(s),..., \hat{a}_N(s))^T \ ,$$

and matrices:

$$H_k(s) = \begin{bmatrix} Ks\eta & W_1 & . & . & . & . & W_{N-1} & W_N \\ D_{10} & D_{11} & . & . & . & . & D_{1(N-1)} & D_{1N} \\ D_{20} & D_{21} & . & . & . & . & D_{2(N-1)} & D_{2N} \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ D_{(N-1)0} & D_{(N-1)1} & . & . & . & . & D_{(N-1)(N-1)} & D_{(N-1)N} \\ Q_N & Q_{N-1} & . & . & . & . & Q_1 & ks\eta \end{bmatrix}$$

$$E = \begin{bmatrix} 0 & 0 & . & . & . & . & 0 & 0 \\ B_{10} & B_{11} & . & . & . & . & B_{1(N-1)} & B_{1N} \\ B_{20} & B_{21} & . & . & . & . & B_{2(N-1)} & B_{2N} \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ B_{(N-1)0} & B_{(N-1)1} & . & . & . & . & B_{(N-1)(N-1)} & B_{(N-1)N} \\ 0 & 0 & . & . & . & . & 0 & 0 \end{bmatrix}$$

We have matrices form of (16), (17) and (18) as follows:

$$H_k(s)\hat{a}(s) = E\,a(0) \ , \qquad (19)$$

Where $H_k(s), E$ are matrices in order $(N+1)\times(N+1)$. Uniqueness of the solution (19) is a consequence of the following theorem.

3.1. Theorem: If f completely monotone but not constant on $[0,\infty]$, then the function $x \to f(\| x \|^2)$ is a radial, strictly positive definite function on any inner-product space. Thus, for any n distinct points $x_1, x_2, ..., x_n$ in such a space the matrix $A_{ij} = f(\| x_i - x_j \|^2)$ is positive definite (and therefore nonsingular) [7].

We can obtain the corresponding system of (19) which involves $(N+1)$ equations and $(N+1)$ unknowns. This system can be solved either a direct method or iteration methods. The next step of our numerical scheme consist of approximation inversion of Laplace transform. We discuss briefly in the following section.

4. The Inversion Formula for the Laplace Transform

The problem of the recovery of a real function $u(t)$, $t > 0$, given its Laplace transform [12]:

$$U(s) = \int_0^\infty e^{-st} u(t)\, dt \quad ,$$

for real values of s, is an ill-posed problem in the sense of Hadamard and is therefore affected by numerical instability. This difficulty is not very serious when $U(s)$ is also known for complex values of s. In such a case, several methods have been developed which, in general, work rather well even if they require a large computational cost and high-precision arithmetic. More stable method can be find in [13]. Here, we explain one of the inversion formulae for the calculation of the original function $u(t)$, $t > 0$, and it is called Legendre expansion method [14]. It's shown that of the Laplace transform i.e. $u(t)$ can be formulated, by using Legendre polynomials. If $u(t)$ is defined at each point of the positive real line, then the function:

$$e^{-(h-1)t} u(t) \qquad , \qquad h > 1 \ ,$$

may be expanded as a Fourier-Legendre series:

$$\sum_{n=0}^{\infty} a_n P_n(x) \qquad , \qquad x = 1 - 2e^{-t} \ ,$$

where the coefficients are given by the formula:

$$a_n = (n + \frac{1}{2}) \int_{-1}^{1} u(t)\, e^{-(h-1)t} P_n(x) dx \ ,$$

$$= (2n+1) \int_0^\infty u(t)\, e^{-ht} P_n(1 - 2e^{-t}) dt \ .$$

Making use of Murphy's formula:

$$P_n(x) = \sum_{r=0}^{n} \frac{(-n)_r (n+1)_r}{(r!)^2} (\frac{1-x}{2})^r \ ,$$

we see that:

$$a_n = (2n+1)\sum_{r=0}^{n} \frac{(-n)_r (n+1)_r}{(r!)^2} U(h+r) \quad , h > 1 . \qquad (20)$$

Hence we have the inversion formula:

$$u(t) = e^{(h-1)t} \sum_{n=0}^{\infty} a_n P_n (1 - 2e^{-t}) \quad ,$$

with the coefficients a_n given by the formula (20). This formula is useful when the transform U is known at a discrete set of points.

5. Numerical Results

Example 1. Consider initial value problem of Schrodinger equation as follows:

$$i\frac{\partial u}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + u(x,t) - e^{-t}(3+3i) + (9+7i)x - 6x^2 - 6ix^3 + 2ix^4 \quad , 0 \le x \le 1 \ , t > 0 \ ,$$

$$\frac{\partial u}{\partial x}(0,t) = \int_0^t \frac{du(0,\mu)}{d\mu} \frac{1}{\sqrt{t-\mu}} d\mu + (1+i)\, e^{-t} \ , \quad t > 0 \ ,$$

$$\frac{\partial u}{\partial x}(1,t) = -\int_0^t \frac{du(1,\mu)}{d\mu} \frac{1}{\sqrt{t-\mu}} d\mu \ , \quad t > 0 \ ,$$

$$u(x,0) = (1+i)(1-x)^3 x \quad , \qquad 0 \le x \le 1 .$$

It's analytic solution :

$$u(x,t) = (1+i)(1-x)^3 x e^{-t} \quad .$$

We take number of nodes 7 and bases function as follows:

$$\psi_i(x) = \sqrt{(x-x_i)^2 + 1} \ .$$

We can see that corresponding error is:

$$\left\| U(x,s) - U^h(x,s) \right\|_\infty = 0.003 .$$

Example 2. Consider initial value problem of Schrodinger equation as follows**:**

$$i\frac{\partial u}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + x\,u(x,t) - e^{-t}(1+i)(1 + ix + (1-i)x^2 - x^3) \quad , 0 \le x \le 1 \ , t > 0 \ ,$$

$$\frac{\partial u}{\partial x}(0,t) = \int_0^t \frac{du(0,\mu)}{d\mu} \frac{1}{\sqrt{t-\mu}} d\mu + (1+i)\, e^{-t} \ , \quad t > 0 \ ,$$

$$\frac{\partial u}{\partial x}(1,t) = -\int_0^t \frac{du(1,\mu)}{d\mu} \frac{1}{\sqrt{t-\mu}} d\mu - (1+i)e^{-t} \ , \quad t > 0 \ ,$$

$$u(x,0) = (1+i)(1-x)x \quad , \qquad 0 \le x \le 1 .$$

It's analytic solution :

$$u(x,t) = (1+i)(1-x)xe^{-t} \quad .$$

We take number of nodes 7 and bases function as follows:

$$\psi_i(x) = \sqrt{(x-x_i)^2 + 1} \ .$$

We can see that corresponding error is:

$$\left\| U(x,s) - U^h(x,s) \right\|_\infty = 0.00054 .$$

6. Conclusion

In this paper, we have presented a scheme to obtain a numerical solution of the Schrodinger equation with TBCs using collocation method. The results reported here show that the collocation method based on RBF has many advantages as compared with other methods such as finite difference method and finite element method. Finite difference methods can be made high-order accurate, but require a structured grid. Finite element methods are highly flexible, but it is hard to achieve high-order accuracy, and both coding and mesh generation become increasingly difficult when the number of space dimensions increases. The most powerful feature of our scheme is flexibility of implementation and application. The numerical scheme consists of two parts, collocation method and Laplace transform method. Both methods are ill-condition. To stabilize the collocation method, we may use RBFs by compact support. Recently, more stable methods recommended by investigators. On the other hand, we can obtain approximation function and it is easy to generalize this method to higher dimension.

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