

# A NUMERICAL METHOD FOR 1D TIME-DEPENDENT SCHRÖDINGER EQUATION USING RADIAL BASIS FUNCTIONS\*

TONGSONG JIANG and ZHAOLIN JIANG

*Department of Mathematics, Linyi Normal University  
 Linyi, Shandong, 276005, P. R. China*

JOSEPH KOLIBAL<sup>†</sup>

*Department of Mathematics, University of Southern Mississippi  
 Hattiesburg, MS 39406, U.S.A.  
 joseph.kolibal@usm.edu*

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This paper proposes a new numerical method to solve the 1D time-dependent Schrödinger equations based on the finite difference scheme by means of multiquadrics (MQ) and inverse multiquadrics (IMQ) radial basis functions. The numerical examples are given to confirm the good accuracy of the proposed methods.

*Keywords:* 1D Schrödinger equation; finite difference; radial basis functions.

## 1. Introduction

The time-dependent Schrödinger equations are very important equations and have been widely used in quantum mechanics, quantum chemistry, optics, electromagnetic wave propagation, underwater acoustics and seismology. In this paper, we consider the following initial value problem of the 1D time-dependent Schrödinger equation:

$$-i\frac{\partial u(x,t)}{\partial t} = \alpha\frac{\partial^2 u(x,t)}{\partial x^2} - \omega(x,t)u(x,t), \quad \forall (x,t) \in \mathbb{R} \times (0,T], \quad (1)$$

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<sup>†</sup>Corresponding author.

$$u(x, 0) = f(x), \quad \forall x \in \mathbb{R}, \quad (2)$$

in which  $\omega(x, t)$  is the potential (real valued) function given on  $\mathbb{R} \times (0, T]$ ,  $f(x)$  is a complex initial data given on  $\mathbb{R}$ , the unknown function  $u(x, t)$  is a complex valued function on  $\mathbb{R} \times (0, T]$ , and  $\alpha$  is a constant.

There have been attempts to develop numerical schemes for (1) and (2) based on finite difference and finite element methods [Antoine and Besse (2003); Han *et al.* (2005); Jin and Wu (2008)]. The authors studied the theoretical analysis of a fully discrete scheme and the problems of the construction of stable approximation schemes for the 1D linear Schrödinger equation on an unbounded domain by reducing the original problem into an initial boundary value problem in a bounded domain with a transparent boundary condition. Artificial boundary conditions are introduced to reduce the original problem to an initial boundary value problem on a finite computational domain, and some unconditionally stable discretization schemes are developed for these kinds of problems. These schemes are proven to be unconditionally stable and convergent, and numerical examples show the effectiveness of the different schemes.

Finite difference methods are the first techniques for solving partial differential equations [Dehghan (2006)]. Even though these methods are very effective, the conditional stability of explicit finite-difference procedures, or the need to use large amount of CPU time in implicit finite difference schemes limit [Dehghan and Tatari (2006)] the applicability of these methods. Furthermore, the accuracy of the techniques is reduced in nonsmooth and nonregular domains. Finite-element procedures have been used as an alternative method to numerical solution of partial differential equations. This family of numerical schemes is efficient specially for solving problems with arbitrary geometry but the need to produce a body-fitted mesh in two- and three-dimensional problems makes these methods quite time-consuming and difficult to use [Chantrasirivan (2004)]. Overall, finite element techniques are highly flexible, but it is hard to obtain results with high-order accuracy.

To avoid difficulty with mesh generation, meshless techniques have attracted the attention of researchers in recent years. In a meshless (meshfree) method a set of scattered nodes are used instead of meshing the computational domain. Meshless schemes include the element-free Galerkin method, the reproducing kernel particle, and local point interpolation [Liu and Gu (2004)]. Over the last 20 years, radial basis functions (RBFs) methods are described as powerful tools for scattered data interpolation problems [Zerroukat *et al.* (1992); Buhmann (2003)]. The use of radial basis functions as a meshless procedure for the numerical solution of partial differential equations is based on a collocation scheme, so that this method does not need to evaluate any integrals. The advantage of radial basis functions over traditional techniques is the meshless property of these methods for solving partial differential equations. This paper presents a new numerical scheme to solve the 1D time-dependent Schrödinger equation by means of finite difference and RBFs.

## 2. Radial Basis Function Interpolation

Consider the interpolation of a multivariate function  $f : \Omega \rightarrow \mathbb{R}$ , where  $\Omega \subset \mathbb{R}$ , from a set of sample values  $\{f(\mathbf{x}_j)\}_{j=1}^N$  on a discrete set  $X = \{\mathbf{x}_j\}_{j=1}^N \subset \Omega$ . Such multivariate functions can be efficiently reconstructed if they are approximated by linear combinations of univariate interpolation functions with Euclidean norm  $\|\cdot\|$ . This can be achieved by using translates  $\Phi(\mathbf{x} - \mathbf{x}_j)$  of a single continuous real valued function  $\Phi$  defined on  $\mathbb{R}$ , and by letting  $\Phi$  be radially symmetric; i.e.,

$$\Phi(\mathbf{x}) := \varphi(\|\mathbf{x}\|),$$

with a continuous function  $\varphi$  on  $\mathbb{R}_0^+$ . In the mathematical literature,  $\varphi$  is often called a RBF with centers  $\{\mathbf{x}_j\}_{j=1}^N$  and  $\Phi$  is the associate kernel.

Interpolants  $\hat{f}_N$  to  $f$  can be constructed as

$$\hat{f}_N(\mathbf{x}) = \sum_{j=1}^N a_j \varphi(r_j) \quad (3)$$

in which  $r_j = \|\mathbf{x} - \mathbf{x}_j\|$ , with real coefficients  $\{a_j\}_{j=1}^N$ . The coefficients on the right-hand side of (3) can be determined by interpolation

$$\hat{f}_N(\mathbf{x}_i) = f(\mathbf{x}_i), \quad 1 \leq i \leq N,$$

provided that the linear system

$$\sum_{j=1}^N a_j \varphi(r_{ij}) = f(\mathbf{x}_i), \quad r_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|, \quad 1 \leq i \leq N, \quad (4)$$

is uniquely solvable. This is true if the symmetric  $N \times N$  matrix

$$A_\varphi = \begin{pmatrix} \varphi(r_{11}) & \cdots & \varphi(r_{1n}) \\ \vdots & \ddots & \vdots \\ \varphi(r_{n1}) & \cdots & \varphi(r_{nn}) \end{pmatrix} \quad (5)$$

is nonsingular.

The most widely used RBFs are

Multiquadric (MQ),	$\varphi(r_j) = \sqrt{r_j^2 + c^2},$
Inverse multiquadric (IMQ),	$\varphi(r_j) = 1/\sqrt{r_j^2 + c^2},$
Inverse quadric (IQ),	$\varphi(r_j) = 1/(r_j^2 + c^2),$
Thin plate spline (TPS),	$\varphi(r_j) = r_j^2 \log(r_j),$
Gaussian (G),	$\varphi(r_j) = e^{-c^2 r_j^2}.$

In the RBF literatures [Buhmann (2003); Micchelli (1986)], it has been observed that, for certain choices of RBFs, (5) could be singular for some configurations of interpolation points. As a result, a lot of interest arose in finding sufficient conditions to ensure the existence of  $A_\varphi^{-1}$  [Buhmann (2003)].

Most of the globally defined RBFs are only conditionally positive definite [Micchelli (1986)]. The unique solvability of the interpolation problem can be obtained by adding a polynomial term to the interpolation (3), giving

$$\hat{f}_N(\mathbf{x}) = \sum_{j=1}^N a_j \varphi(r_j) + \sum_{k=1}^K b_k p_k(\mathbf{x}), \quad (6)$$

along with the constraints

$$\sum_{j=1}^N a_j p_k(\mathbf{x}_j) = 0, \quad 1 \leq k \leq K, \quad (7)$$

where  $\{p_k\}_{k=1}^K$  is a basis for  $\mathcal{P}_{m-1}$ , the set of polynomials in one variable of degree  $\leq m-1$ , and

$$t = \binom{m+1}{2}$$

is the dimension of  $\mathcal{P}_{m-1}$ . Let

$$P^T = \begin{pmatrix} p_1(\mathbf{x}_1) & \cdots & p_1(\mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ p_t(\mathbf{x}_1) & \cdots & p_t(\mathbf{x}_N) \end{pmatrix}.$$

The interpolation conditions  $f(\mathbf{x}_i) = \sum_{j=1}^N a_j \varphi(r_{ij}) + \sum_{k=1}^K b_k p_k(\mathbf{x}_i)$ ,  $1 \leq i \leq N$ , subject to (7) can be rewritten as the linear system

$$\begin{pmatrix} A_\varphi & P \\ P^T & 0 \end{pmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix}, \quad (8)$$

where  $\mathbf{a} = [a_1, \dots, a_N]^T$ ,  $\mathbf{b} = [b_1, \dots, b_K]^T$  and  $\mathbf{f} = [f(\mathbf{x}_1), \dots, f(\mathbf{x}_N)]^T$ .

In the last decade, the development of RBFs as a truly meshless method for approximating the solutions of PDEs has drawn the attention of many researchers in science and engineering. One of the domain-type meshless methods, the so-called Kansas method developed by Kansa [1990a, 1990b], is obtained by directly collocating the RBFs, particularly the MQ and IMQ, for the numerical approximation of the solution. Kansas' method was recently extended to solve various ordinary and partial differential equations including the 1D nonlinear Burgers equation [Hon and Mao (1998)] with shock wave, shallow water equations for tide and currents simulation [Hon *et al.* (1999)], heat transfer problems [Zerroukat *et al.* (1992)], and free boundary problems [Hon and Mao (1999); Marcozzi *et al.* (2001)].

### 3. Methodology

Consider (1) and (2) on a finite interval  $[a, b]$ , on which  $u(x, t)$  satisfies the following one-dimensional time-dependent Schrödinger equation

$$-i \frac{\partial u(x, t)}{\partial t} = \alpha \frac{\partial^2 u(x, t)}{\partial x^2} - \omega(x, t) u(x, t), \quad \forall (x, t) \in [a, b] \times (0, T), \quad (9)$$

with the initial condition

$$u(x, 0) = f(x), \quad \forall x \in [a, b], \quad (10)$$

and the measured Dirichlet boundary condition

$$u(x, t) = g(x, t), \quad \forall (x, t) \in [a, b] \times (0, T], \quad (11)$$

in which  $\omega(x, t)$  is the potential (real valued) function given on  $[a, b] \times (0, T]$ ,  $f(x)$  and  $g(x, t)$  are known complex functions on  $[a, b]$ , the unknown function  $u(x, t)$  is a complex valued function on  $[a, b] \times (0, T]$ , and  $\alpha$  is a constant.

In the following section, a generalized trapezoidal method ( $\theta$ -method) is used to approximate the time derivative in (9). Let  $\delta t = t^{n+1} - t^n$  be the time step and  $t^n = n\delta t$ , be the mesh in time direction. For any  $t^n \leq t \leq t^{n+1}$  and  $0 \leq \theta \leq 1$ , approximate  $u(x, t)$  by following formulation

$$u(x, t) \simeq \theta u(x, t^{n+1}) + (1 - \theta)u(x, t^n), \quad (12)$$

so that

$$\Delta u(x, t) \simeq \theta \Delta u(x, t^{n+1}) + (1 - \theta)\Delta u(x, t^n), \quad (13)$$

and

$$\frac{\partial u(x, t)}{\partial t} \simeq \frac{u(x, t^{n+1}) - u(x, t^n)}{\delta t}, \quad (14)$$

in which  $\Delta = \partial^2 / \partial x^2$ . For simplicity, we denote  $u^n(x) \equiv u(x, t^n)$ . Substituting (13) and (14) to our problem (9)–(11), we obtain the following equation

$$\begin{aligned} -i \frac{u^{n+1}(x) - u^n(x)}{\delta t} &= \theta [\alpha \Delta u^{n+1}(x) - \omega(x, t)u^{n+1}(x)] \\ &\quad + (1 - \theta) [\alpha \Delta u^n(x) - \omega(x, t)u^n(x)]. \end{aligned} \quad (15)$$

Rewrite (15) as

$$-iu^{n+1} - \theta \delta t [\alpha \Delta u^{n+1} - \omega(x, t)u^{n+1}] = -iu^n - (1 - \theta) \delta t [\alpha \Delta u^n - \omega(x, t)u^n]. \quad (16)$$

Uniformly choose  $p$  collocation points  $\{\mathbf{x}_i\}_{i=1}^{n_I}$  in the interior of domain  $[a, b]$  and two boundary points  $[a, 0]$  and  $[b, 0]$  with  $N = p + 2$ .

Let  $u^n(x)$  be approximated by

$$u^n(x) \simeq \sum_{j=1}^N \lambda_j^n \varphi_j(r_{ij}), \quad (17)$$

where  $r_{ij} = \sqrt{(x_i - x_j)^2}$ ,  $i, j = 1, 2, \dots, N$ . In this paper, we mainly use multi-quadratics and inverse multi-quadratics radial basis functions

$$\varphi_1(r) = \sqrt{r^2 + c^2}, \quad \varphi_2(r) = \frac{1}{\sqrt{r^2 + c^2}},$$

with

$$\frac{\partial^2 \varphi_1(r)}{\partial x^2} = \frac{c^2}{\sqrt{(r^2 + c^2)^3}}, \quad \frac{\partial^2 \varphi_2(r)}{\partial x^2} = -\frac{1}{\sqrt{(r^2 + c^2)^3}} + \frac{3r^2}{\sqrt{(r^2 + c^2)^5}}.$$

Write (17) together with boundary condition (11) in a matrix form as

$$[u]^n = A[\lambda]^n, \quad (18)$$

where  $[u]^n = [u_1^n, u_2^n, \dots, u_N^n]^T$ ,  $[\lambda]^n = [\lambda_1^n, \lambda_2^n, \dots, \lambda_N^n]^T$  and  $A = (a_{ij})$ ,  $1 \leq i, j \leq N$ . Assuming that there are  $p < N$  internal points and  $N - p$  boundary points, the  $N \times N$  matrix  $A$  can be split into  $A = A_d + A_b$ , in which

$$A_d = \begin{cases} (a_{ij}), & \text{if } 1 \leq i \leq p, \ 1 \leq j \leq N \\ a_{ij} = 0, & \text{otherwise} \end{cases},$$

$$A_b = \begin{cases} a_{ij}, & \text{if } p+1 \leq i \leq N, \ 1 \leq j \leq N \\ a_{ij} = 0, & \text{otherwise} \end{cases}.$$

Then (16) together with (11) can be written, by applying to the domain points and boundary points, in a following matrix form:

$$(-iA_d + B)[\lambda]^{n+1} = (-iA_d + C)[\lambda]^n + [g]^{n+1}, \quad (19)$$

in which

$$B = -\theta\delta t(\alpha\Delta A_d - \omega \otimes A_d) + A_b, \quad C = (1 - \theta)\delta t(\alpha\Delta A_d - \omega \otimes A_d), \quad (20)$$

$$\omega = [\omega_1 \ \cdots \ \omega_p \ 0 \ 0]^T, \quad [g]^l = [0 \ \cdots \ 0 \ g_{p+1}^n \ g_N^n]^T, \quad (21)$$

and the symbol " $\omega \otimes A_d$ " means that  $i$ th component of vector  $\omega$  is multiplied on all components of  $i$ th row of matrix  $A_d$ .

Let  $[\lambda]^n = [\text{Re}(\lambda)]^n + [\text{Im}(\lambda)]^n i$  and  $[g]^n = [\text{Re}(g)]^n + [\text{Im}(g)]^n i$ . Then (19) is equivalent to

$$\begin{pmatrix} B & A_d \\ -A_d & B \end{pmatrix} \begin{bmatrix} \text{Re}(\lambda) \\ \text{Im}(\lambda) \end{bmatrix}^{n+1} = \begin{pmatrix} C & A_d \\ -A_d & C \end{pmatrix} \begin{bmatrix} \text{Re}(\lambda) \\ \text{Im}(\lambda) \end{bmatrix}^n \begin{bmatrix} \text{Re}(g) \\ \text{Im}(g) \end{bmatrix}^{n+1}. \quad (22)$$

Therefore the solution of the complex system (22) is reduced to the solution of a real system. Note that the coefficient matrix of Eq. (22) is not changed.

**Remark.** Equation (22) is valid for any of  $\theta \in [0, 1]$ , the method is called implicit Euler method if  $\theta = 1$  and the method is called Crank–Nicolson method if  $\theta = 1/2$ .

## 4. Numerical Examples

In this section, we present two examples to show the effectiveness and accuracy of proposed scheme. In order to evaluate the numerical errors, we adopt the maximum error as defined by

$$E_m = \max_{(x,t) \in \{x_k, t_k\}} |u(x, t) - U(x, t)|, \quad (23)$$

where  $u(x, t)$  is the exact analytical solution, and  $U(x, t)$  is the numerical solution at  $(x, t)$ .

### 4.1. Example 1

Consider the following 1D time-dependent Schrödinger equation with the domain square  $[-5, 5]$  with a vanishing potential

$$-i\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2} - \omega(x, t)u(x, t), \quad (24)$$

It is well known that an exact solution is given in Antoine and Besse [2003] as

$$u(x, t) = \sqrt{\frac{i}{i - 4t}} \exp\left(\frac{-ix^2 - k_0x + k_0^2t}{i - 4t}\right). \quad (25)$$

Using an initial condition

$$u(x, 0) = \exp(-x^2 + k_0xi),$$

the boundary conditions can be found from the exact solution (24) as

$$\begin{aligned} u(-5, t) &= \sqrt{\frac{i}{i - 4t}} \exp\left(\frac{-25i + 5k_0 + k_0^2t}{i - 4t}\right), \\ u(5, t) &= \sqrt{\frac{i}{i - 4t}} \exp\left(\frac{-25i - 5k_0 + k_0^2t}{i - 4t}\right). \end{aligned}$$

In this example we take two radial basis functions MQ and IMQ and  $k_0 = 8, dx = 0.05, dt = 10^{-6}$ . In Table 1 we report the maximum errors with the implicit Euler method ( $\theta = 1$ ) and the Crank–Nicolson method ( $\theta = 1/2$ ) and two radial basis functions MQ ( $c = 0.30$ ) and IMQ ( $c = 0.40$ ) at different times  $T$ . In Figs. 1–3 the evolution of the exact solution and the numerical solutions at different times are shown graphically for the MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1$ ), respectively. It can be seen from these figures that the proposed method performs well.

Table 1. Maximum errors with the implicit Euler method ( $\theta = 1$ ) and the Crank–Nicolson method ( $\theta = 1/2$ ) and two RBFs MQ ( $c = 0.30$ ) and IMQ ( $c = 0.40$ ) at different times  $T$  for  $k_0 = 8, dx = 0.05, dt = 10^{-6}$ .

Method	Implicit Euler		Crank–Nicolson	
RBFs	$E_m(\text{MQ})$	$E_m(\text{IMQ})$	$E_m(\text{MQ})$	$E_m(\text{IMQ})$
$T = 0.05$	$1.209 \times 10^{-4}$	$1.209 \times 10^{-4}$	$1.939 \times 10^{-9}$	$1.655 \times 10^{-9}$
$T = 0.15$	$3.428 \times 10^{-4}$	$3.427 \times 10^{-4}$	$7.371 \times 10^{-6}$	$2.865 \times 10^{-6}$
$T = 0.30$	$1.000 \times 10^{-3}$	$6.985 \times 10^{-4}$	$1.044 \times 10^{-3}$	$5.310 \times 10^{-4}$
$T = 0.45$	$4.803 \times 10^{-4}$	$1.708 \times 10^{-4}$	$8.707 \times 10^{-4}$	$4.497 \times 10^{-4}$
$T = 0.60$	$4.333 \times 10^{-4}$	$1.558 \times 10^{-4}$	$7.840 \times 10^{-4}$	$4.005 \times 10^{-4}$
$T = 0.80$	$5.732 \times 10^{-4}$	$2.714 \times 10^{-4}$	$1.086 \times 10^{-3}$	$5.442 \times 10^{-4}$
$T = 1.00$	$5.795 \times 10^{-4}$	$1.518 \times 10^{-4}$	$1.001 \times 10^{-3}$	$5.381 \times 10^{-4}$

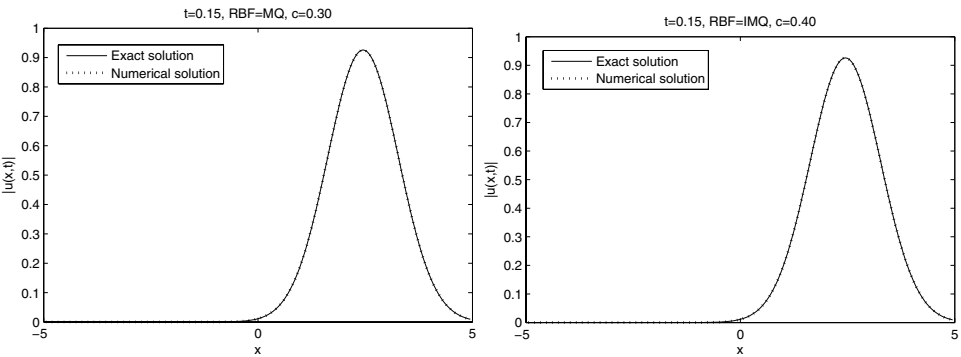


Fig. 1. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1$ ) at time  $t = 0.15$  for example problem 1.

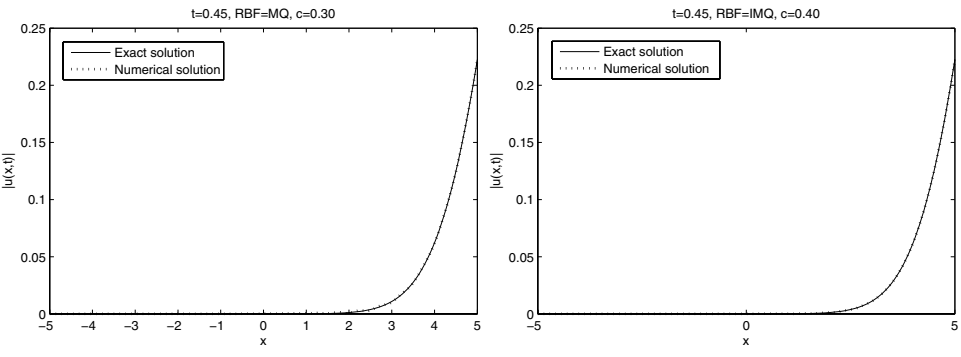


Fig. 2. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1$ ) at time  $t = 0.45$  for example problem 1.

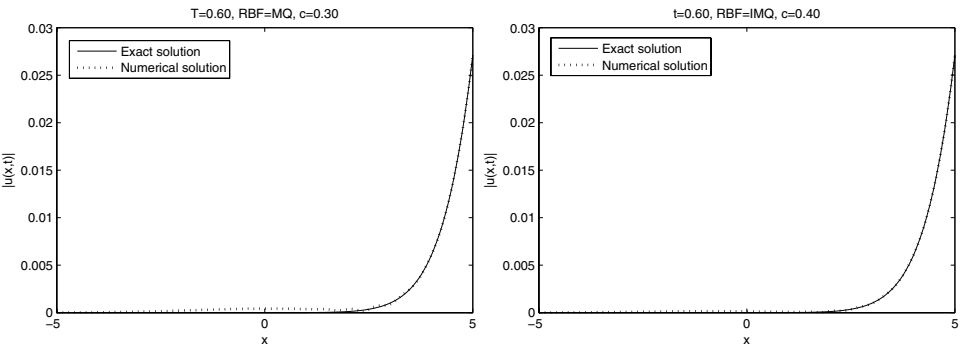


Fig. 3. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1$ ) at time  $t = 0.60$  for example problem 1.



## 4.2. Example 2

Consider the 1D time-dependent Schrödinger equation with the domain  $[0, 1]$  with a potential  $\omega(x, t) = 1$ . Satisfying

$$-i \frac{\partial u(x, t)}{\partial t} = \frac{1}{2} \frac{\partial^2 u(x, t)}{\partial x^2} - \omega(x, t)u(x, t). \quad (26)$$

An exact solution of (26) is given in Jin and Wu [2008] as

$$u(x, t) = \sqrt{\frac{i}{i - 200t}} \exp \left( \frac{i(200t^2 - (10x - 5)^2) - k_0(10x - 5) + (50k_0^2 + 1)t}{i - 200t} \right). \quad (27)$$

Setting the initial condition to,

$$u(x, 0) = \exp(-(10x - 5)^2 + k_0(10x - 5)i), \quad (28)$$

the boundary conditions can be found from the exact solution as

$$u(0, t) = \sqrt{\frac{i}{i - 200t}} \exp \left( \frac{i(200t^2 - 25) + 5k_0 + (50k_0^2 + 1)t}{i - 200t} \right), \quad (29)$$

$$u(1, t) = \sqrt{\frac{i}{i - 200t}} \exp \left( \frac{i(200t^2 - 25) - 5k_0 + (50k_0^2 + 1)t}{i - 200t} \right). \quad (30)$$

In this example, we take two RBFs MQ and IMQ and  $k_0 = 8, dx = 0.01, dt = 5 \times 10^{-8}$ . In Table 2 we report the maximum errors with the implicit Euler method ( $\theta = 1$ ) and the Crank–Nicolson method ( $\theta = 1/2$ ) and two RBFs MQ ( $c = 0.05$ ) and IMQ ( $c = 0.08$ ) at different times  $T$ . In Figs. 4–8 the evolution of the exact solution and the numerical solutions at different times are shown graphically for the MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ), respectively. It can be seen from these figures that the proposed method performs well.

Table 2. Maximum errors with the implicit Euler method ( $\theta = 1$ ) and the Crank–Nicolson method ( $\theta = 1/2$ ) and two RBFs MQ ( $c = 0.05$ ) and IMQ ( $c = 0.08$ ) at different times  $T$  for  $k_0 = 8, dx = 0.01, dt = 5 \times 10^{-8}$ .

Method	Implicit Euler		Crank–Nicolson	
RBFs	$E_m(\text{MQ})$	$E_m(\text{IMQ})$	$E_m(\text{MQ})$	$E_m(\text{IMQ})$
$T = 0.001$	$3.024 \times 10^{-4}$	$3.024 \times 10^{-4}$	$1.095 \times 10^{-8}$	$1.039 \times 10^{-8}$
$T = 0.003$	$8.571 \times 10^{-4}$	$8.571 \times 10^{-4}$	$7.865 \times 10^{-5}$	$2.774 \times 10^{-5}$
$T = 0.005$	$6.697 \times 10^{-3}$	$4.282 \times 10^{-3}$	$7.272 \times 10^{-3}$	$2.701 \times 10^{-3}$
$T = 0.007$	$9.137 \times 10^{-3}$	$4.374 \times 10^{-3}$	$9.488 \times 10^{-3}$	$3.516 \times 10^{-3}$
$T = 0.009$	$8.136 \times 10^{-3}$	$3.800 \times 10^{-3}$	$8.690 \times 10^{-3}$	$3.218 \times 10^{-3}$
$T = 0.012$	$7.310 \times 10^{-3}$	$3.392 \times 10^{-3}$	$7.800 \times 10^{-3}$	$2.874 \times 10^{-3}$
$T = 0.015$	$8.433 \times 10^{-3}$	$4.311 \times 10^{-3}$	$8.952 \times 10^{-3}$	$3.552 \times 10^{-3}$

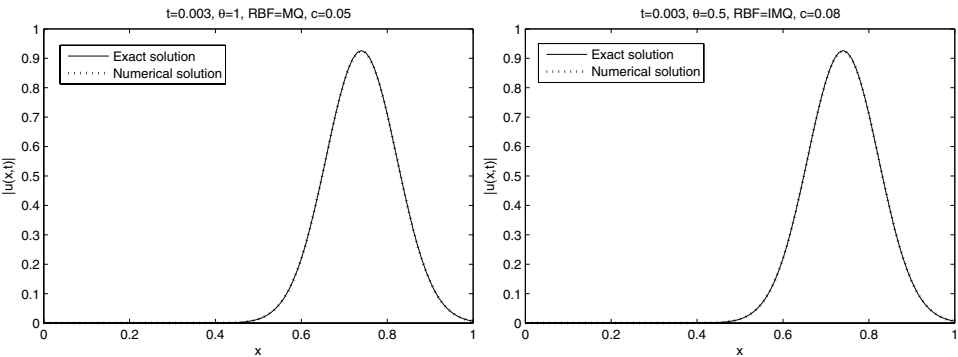


Fig. 4. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ) at time  $t = 0.003$  from example problem 2.

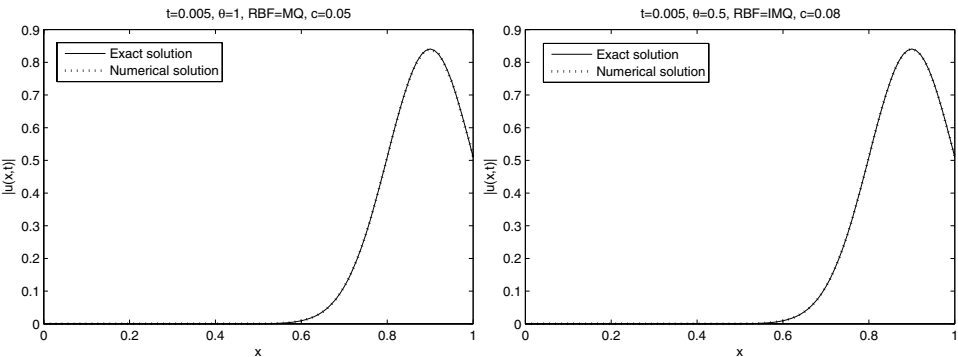


Fig. 5. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ) at time  $t = 0.005$  from example problem 2.

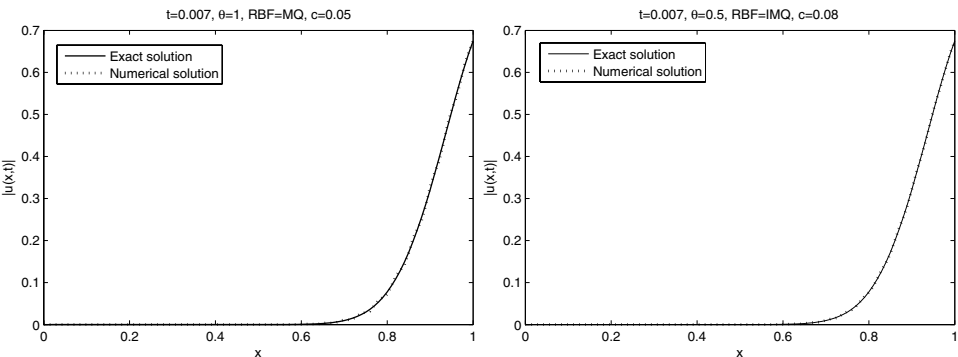


Fig. 6. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ) at time  $t = 0.007$  from example problem 2.

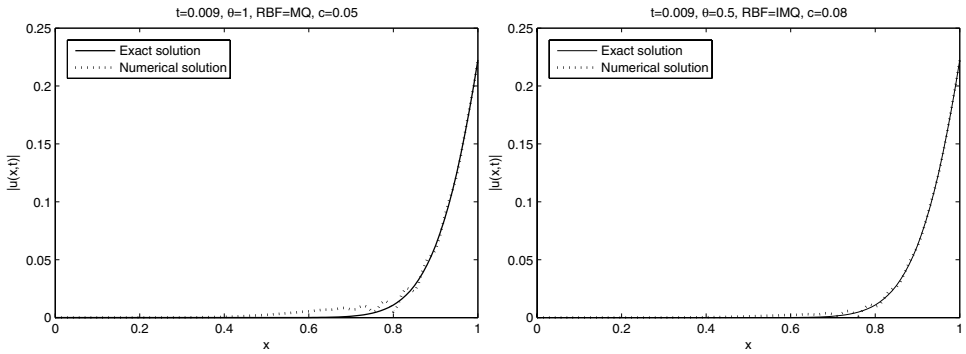


Fig. 7. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ) at time  $t = 0.009$  from example problem 2.

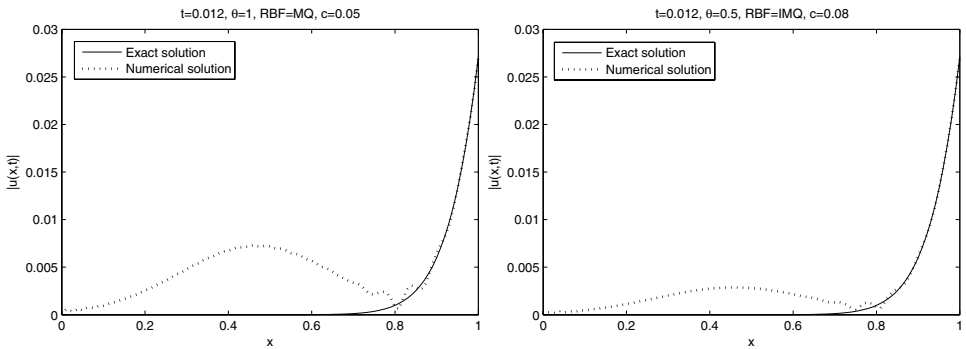


Fig. 8. Comparisons of numerical solutions and exact solutions with MQ ( $\theta = 1$ ) and IMQ ( $\theta = 1/2$ ) at time  $t = 0.012$  from example problem 2.

## 5. Conclusion

In this paper, we proposed a new numerical method to solve the 1D time-dependent Schrödinger equation by means of finite difference in time and RBF with MQ and IMQ. The effectiveness of the proposed computational scheme is well demonstrated by several examples.

It has to be emphasized that the choice of RBFs is a flexible feature of meshless methods. The RBFs can be globally supported, infinitely differentiable and contain free parameters that is called shape parameters, which affect both accuracy of the solutions and conditioning of the collocation matrix. The shape parameters in Examples 1 and 2 with MQ and IMQ for all the calculations performed in this paper were found experimentally. The optimal choice of the shape parameters in RBF is still under investigation.

In addition, for certain choices of RBFs, the resulting matrix could be singular for some configurations of interpolation points and the system may also be

ill-conditioned. To order to guarantee the unique solvability of the interpolation problem, one can use compact support RBFs or preconditioning methods by add a polynomial term to the interpolation.

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