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An Alternating Group Iterative Method for Schrodinger Equations

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Abstract

Based on four saul'yev asymmetry iterative schemes we construct a class of alternating group iterative method with intrinsic parallelism for schrodinger equations. The method is verified to be convergent. Results of the numerical experiments show that the method is of higher accuracy.

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1 Introduction

In scientific and engineering computing, we usually need to solve large equation set by numerical methods. Considering the stability and accuracy of explicit schemes and the computation difficulty of implicit schemes, it is necessary to construct methods with the advantages of explicit methods and implicit methods, that is, simple for computation and good stability. Based on the concept of domain decomposition, D. J. Evans presented a class of AGE method in [1], which has the advantages of unconditional stability and parallelism. The AGE method is soon applied to convection-diffusion equations and hyperbolic equations in [2,3]. In [4-5], AGE methods are applied for two-point linear and non-linear boundary value problems.

In this paper, we will consider the following initial boundary value problem of schrodinger equations:

$$\begin{cases} \frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2},\ 0 \le x \le 1,\ 0 \le t \le T \\ u(x,0) = f(x), \\ u(0,t) = g_1(t),\ u(1,t) = g_2(t). \end{cases} \quad (1)$$

Many finite difference methods on schrodinger equations have been presented[6-8], but to our knowledge AGE methods for schrodinger equations have scarcely been presented.

We organize the rest of this paper as follows:

In section 2, we present a $O(\tau^2+h^4)$ order unconditionally stable symmetry six-point implicit scheme for solving (1) at first. Based on the scheme we present a group of saul'yev asymmetry iterative schemes, and then a class of alternating group explicit iterative method is constructed. Convergence analysis is given in section 3. In order to verify the method, results of numerical example are presented at the end of the paper.

2 The Alternating Group Iterative Method

The domain $\Omega : [0,1] \times [0,T]$ will be divided into $(m \times N)$ meshes with spatial step size h=$\frac{1}{m}$ in x direction and the time step size τ=$\frac{T}{N}$. Grid points are denoted by (x_i, t_n) or (i, n), $x_i = ih(i = 0,\ 1, \cdots, m),\ t_n = n\tau(n = 0,\ 1, \cdots, \frac{T}{\tau})$. The numerical solution of (1) is denoted by u_i^n, while the exact solution $u(x_i,\ t_n)$. Let $r = \frac{\tau}{h^2}$.

We present an implicit unconditionally stable finite difference scheme with accurate of order $O(\tau^2 + h^4)$ for solving (1) as below:

$$(1-6ri)u_{i-1}^{n+1}+(10+12ri)u_i^{n+1}+(1-6ri)u_{i+1}^{n+1} = (1+6ri)u_{i-1}^n+(10-12ri)u_i^n+(1+6ri)u_{i+1}^n \quad (2)$$

Let $E_i^n = (1 + 6ri)u_{i-1}^n + (10 - 12i)u_i^n + (1 + 6ri)u_{i+1}^n,\ a_1 = 5 + 6ri,\ a_2 = \frac{1}{2}(1 - 6ri)$. Then (2) can be rewritten as:

$$2a_2u_{i-1}^{n+1} + 2a_1u_i^{n+1} + 2a_2u_{i+1}^{n+1} = E_i^n \quad (3)$$

In order to get the numerical solution of (n+1)-th time level with the solution of n-th time level known, we will present four asymmetry iterative schemes. k denotes the iterative number.

$$(\rho+a_1)u_i^{n+1(k+1)} + a_2u_{i+1}^{n+1(k+1)} = -2a_2u_{i-1}^{n+1(k)} + (\rho-a_1)u_i^{n+1(k)} - a_2u_{i+1}^{n+1(k)} + E_i^n \quad (4)$$

$$a_2u_{i-1}^{n+1(k+1)} + (\rho+a_1)u_i^{n+1(k+1)} + 2a_2u_{i+1}^{n+1(k+1)} = -a_2u_{i-1}^{n+1(k)} + (\rho-a_1)u_i^{n+1(k)} + E_i^n \quad (5)$$

$$2a_2u_{i-1}^{n+1(k+1)} + (\rho+a_1)u_i^{n+1(k+1)} + a_2u_{i+1}^{n+1(k+1)} = (\rho-a_1)u_i^{n+1(k)} - a_2u_{i+1}^{n+1(k)} + E_i^n \quad (6)$$

$$a_2 u_{i-1}^{n+1(k+1)} + (\rho + a_1) u_i^{n+1(k+1)} = -a_2 u_{i-1}^{n+1(k)} + (\rho - a_1) u_i^{n+1(k)} - 2a_2 u_{i+1}^{n+1(k)} + E_i^n \tag{7}$$

Considering the implicit scheme (3) costs computation time, we try to divide the computation in all the whole domain into many sub-domains so as to fulfill the parallelism. Based on (4)-(7), we construct three basic computing point groups:

"$\kappa 1$"group: four grid points are involved, and (4), (5), (6), (7) are used respectively. Let $U_i^{n+1(k+1)} = (u_i^{n+1(k+1)}, u_{i+1}^{n+1(k+1)}, u_{i+2}^{n+1(k+1)}, u_{i+3}^{n+1(k+1)})^T$, Then we have

$$(\rho I + A_1) U_i^{n+1(k+1)} = (\rho I - B_1) U_i^{n+1(k)} + \widehat{E}_i^n \tag{8}$$

here $\widehat{E}_i^n = (-2a_2 u_{i-1}^{n+1(k)} + E_i^n, E_i^n, E_i^n, -2a_2 u_{i+4}^{n+1(k)} + E_i^n)^T$,

$$A_1 = \begin{pmatrix} a_1 & a_2 & 0 & 0 \\ a_2 & a_1 & 2a_2 & 0 \\ 0 & 2a_2 & a_1 & a_2 \\ 0 & 0 & a_2 & a_1 \end{pmatrix}, \ B_1 = \begin{pmatrix} a_1 & a_2 & 0 & 0 \\ a_2 & a_1 & 0 & 0 \\ 0 & 0 & a_1 & a_2 \\ 0 & 0 & a_2 & a_1 \end{pmatrix}.$$

Then the numerical solution $u_i^{n+1(k+1)}$, $u_{i+1}^{n+1(k+1)}$, $u_{i+2}^{n+1(k+1)}$, $u_{i+3}^{n+1(k+1)}$ can be obtained in "κ_1" group as below:

$$U_i^{n+1(k+1)} = (\rho I + A_1)^{-1} [(\rho I - B_1) U_i^{n+1(k)} + \widetilde{E}_i^n] \tag{9}$$

"$\kappa 2$"group: two inner points are involved, and (4), (5) are used respectively. Let $\overline{U}_i^{n+1(k+1)} = (u_i^{n+1(k+1)}, u_{i+1}^{n+1(k+1)})^T$, then we have

$$(\rho I + A_2) \overline{U}_i^{n+1(k+1)} = (\rho I - B_2) \overline{U}_i^{n+1(k+1)} + \overline{E}_i^n \tag{10}$$

here $\overline{E}_i^n = (-2a_2 u_{i-1}^{n+1(k)} + E_i^n, -2a_2 u_{i+2}^{n+1(k+1)} + E_i^n)^T$,

$$A_2 = \begin{pmatrix} a_1 & a_2 \\ a_2 & a_1 \end{pmatrix}, \ B_2 = A_2.$$

If we apply κ_2 group to the right two inner points (m-2,n+1),(m-1,n+1), then the solution of $u_{m-1}^{n+1(k+1)}$, $u_{m-1}^{n+1(k+1)}$ can be denoted as below:

$$\overline{U}_{m-2}^{n+1(k+1)} = (\rho I + A_2)^{-1} [(\rho I - B_2) \overline{U}_i^{n+1(k)} + \overline{E}_i^n]. \tag{11}$$

"$\kappa 3$"group: two inner points are involved, and (6), (7) are used respectively. Let $\widetilde{U}_i^{n+1(k+1)} = (u_i^{n+1(k+1)}, u_{i+1}^{n+1(k+1)})^T$, then we have

$$(\rho I + A_3) \widetilde{U}_i^{n+1(k+1)} = (\rho I - B_3) \widetilde{U}_i^{n+1(k+1)} + \widetilde{E}_i^n \tag{12}$$

here $\widetilde{E}_i^n = (-2a_2 u_{i-1}^{n+1(k+1)} + E_i^n, -2a_2 u_{i+2}^{n+1(k)} + E_i^n)^T$,

$$A_3 = A_2, \ B_3 = B_2$$

Thus we have:

$$\widetilde{U}_i^{n+1} = (\rho I + A_3)^{-1}[(\rho I - B_3)B_3\widetilde{U}_i^n + \widetilde{E}_i^n] \tag{13}$$

Let $U^{n+1(k)} = (u_1^{n+1(k)}, u_2^{n+1(k)}, \cdots, u_{m-1}^{n+1(k)})^T$, we construct the AGE iterative method in two cases as follows:

Case 1: Let $m-1 = 4s$, s is an integer. First in order to get the solution of $U^{n+1(k+\frac{1}{2})}$ with $U^{n+1(k)}$ known, we divide all the $(m-1)$ inner grid points into s groups. Four grid points are included in each group, named $(i, n+1), (i+1, n+1), (i+2, n+1), (i+3, n+1)$, and (9) is applied to get the solution of $u_i^{n+1(k+1)}, u_{i+1}^{n+1(k+1)}, u_{i+2}^{n+1(k+1)}, u_{i+3}^{n+1(k+1)},\ i = 4p+1(p = 0, 1, \cdots, \frac{m-5}{4})$.

Second in order to get the solution of $U^{n+1(k+1)}$ with $U^{n+1(k+\frac{1}{2})}$ known, we divide all the grid points into $s+1$ groups. (13) is used to solve $u_1^{n+1(k+1)}$, $u_2^{n+1(k+1)}$, while (11) is used to solve $u_{m-2}^{n+1(k+1)}$, $u_{m-1}^{n+1(k+1)}$. (9) is used to solve $(u_i^{n+1(k+1)}$, $u_{i+1}^{n+1(k+1)}$ $, u_{i+2}^{n+1(k+1)}, u_{i+3}^{n+1(k+1)}),\ i = 4p+3(p = 0, 1, \cdots, \frac{m-9}{4})$.

By alternating use of the asymmetry schemes (9),(11),(13), the computation in the whole domain can be divided into many sub-domains. So the method has the obvious property of parallelism.

We denote the AGE iterative method as follows:

$$\begin{cases} (\rho I + A)U^{n+1(k+\frac{1}{2})} = (\rho I - B)U^{n+1(k)} + E^n \\ (\rho I + B)U^{n+1(k+1)} = (\rho I - A)U^{n+1(k+\frac{1}{2})} + E^n \end{cases} k = 0, 1 \cdots \tag{14}$$

Here ρ is an iterative parameter. E^n is known vectors relevant to the solution of n-th time level.

$$A = diag(A_1, \cdots, A_1)_{(m-1)\times(m-1)},\ B = diag(B_2, \widehat{B}_1, \cdots, \widehat{B}_1, B_3)_{(m-1)\times(m-1)},\ \widehat{B}_1 = A_1.$$

Case 2: Let $m-1 = 4s+2$, s is an integer. First in order to get the solution of $U^{n+1(k+\frac{1}{2})}$ with $U^{n+1(k)}$ known, we divide all the $(m-1)$ inner grid points into $s+1$ groups. (11) is used to solve $u_{m-2}^{n+1}, u_{m-1}^{n+1}$, while the left $4s$ inner grid points are divided into s κ_1 groups, and (9) is applied to get the solution of $u_i^{n+1(k+1)}, u_{i+1}^{n+1(k+1)}, u_{i+2}^{n+1(k+1)}, u_{i+3}^{n+1(k+1)},\ i = 4p+1(p = 0, 1, \cdots, \frac{m-7}{4})$.

Second in order to get the solution of $U^{n+1(k+1)}$ with $U^{n+1(k+\frac{1}{2})}$ known, we still divide all the inner grid points into $s+1$ groups. (13) is used to solve $u_1^{n+1(k+1)}$, $u_2^{n+1(k+1)}$, while (9) is used to solve $(u_i^{n+1(k+1)}$ $,\ u_{i+1}^{n+1(k+1)}, u_{i+2}^{n+1(k+1)}, u_{i+3}^{n+1(k+1)}),\ i = 4p+3(p = 0, 1, \cdots, \frac{m-7}{4})$.

Then we obtain the alternating group iterative method II :

$$\begin{cases} (\rho I + \widetilde{A})U^{n+1(k+\frac{1}{2})} = (\rho I - \widetilde{B})U^{n+1(k)} + E^n \\ (\rho I + \widetilde{B})U^{n+1(k+1)} = (\rho I - \widetilde{A})U^{n+1(k+\frac{1}{2})} + E^n \end{cases} k = 0, 1 \cdots \tag{15}$$

Here

$$\widetilde{A} = diag(A_1, A_1, \cdots, A_1, A_2)_{(m-1)\times(m-1)},\ \widetilde{B} = diag(B_2, \widehat{B}_1, \cdots, \widehat{B}_1, B_1)_{(m-1)\times(m-1)}.$$

3 Convergence Analysis For The Group Iterative Method

Lemma 1 Let $\rho > 0$, and $G + G^T$ is nonnegative, then $(\rho I + G)^{-1}$exists, and

$$\begin{cases} \|(\rho I + G)^{-1}\|_2 \leq \rho^{-1} \\ \|(\rho I - G)(\rho I + G)^{-1}\|_2 \leq 1 \end{cases} \tag{16}$$

From the construction of the matrices we can see that $A,\ B,\ (A+A^T),\ (B+B^T)$ are all nonnegative matrices. Then we have

$$\|(\rho I - A)(\rho I + A)^{-1}\|_2 \leq 1,\ \|(\rho I - B)(\rho I + B)^{-1}\|_2 \leq 1$$

From (6), we can obtain $U^{n+1(k+1)} = HU^{n+1(k)} + (\rho I + B)^{-1}[(\rho I - A)(\rho I + A)^{-1}E^n + E^n]$. Here $H = (\rho I + B)^{-1}(\rho I - A)(\rho I + A)^{-1}(\rho I - B)$ is the growth matrix.

Let $\widetilde{H} = (\rho I + B)H(\rho I + B)^{-1} = (\rho I - A)(\rho I + A)^{-1}(\rho I - B)(\rho I + B)^{-1}$, then $\rho(H) = \rho(\widetilde{H}) \leq \|\widetilde{H}\|_2 \leq 1$, which shows the AGEI method given by (6) is convergent. Then we have:

Theorem 1 The alternating group iterative method I denoted by (14) is convergent.

Analogously we have:

Theorem 1 The alternating group iterative method II denoted by (15) is also convergent.

4 Numerical Experiments

We consider the following problem:

$$\begin{cases} \dfrac{\partial u}{\partial t} = i\dfrac{\partial^2 u}{\partial x^2},\ 0 \leq x \leq 1,\ 0 \leq t \leq T \\ u(x,0) = e^{i2\pi x}, \\ u(0,t) = e^{-it},\ u(1,t) = e^{-it}. \end{cases} \tag{17}$$

The exact solution of (17) is denoted as below:

$$u(x,t) = e^{i(2\pi x - 4\pi^2 t)}$$

Let A.E=$|u_i^n - u(x_i,t_n)|$ and P.E=$100 \times \dfrac{|u_i^n - u(x_i,t_n)|}{u(x_i,t_n)}$ denote maximum absolute error and relevant error of the presented method in this paper respectively. We present the numerical results in table 1:

Table 1: numerical results at $m = 25$

$\tau = 10^{-3}$	$t = 100\tau$	$t = 200\tau$	$t = 500\tau$	$t = 1000\tau$
A.E.	4.188×10^{-4}	4.418×10^{-4}	1.671×10^{-4}	7.928×10^{-5}
P.E.	6.190×10^{-2}	4.678×10^{-2}	2.416×10^{-2}	9.273×10^{-3}
$\tau = 10^{-4}$	$t = 100\tau$	$t = 200\tau$	$t = 500\tau$	$t = 1000\tau$
A.E.	5.777×10^{-5}	2.711×10^{-5}	7.351×10^{-5}	4.385×10^{-6}
P.E.	5.902×10^{-3}	2.746×10^{-3}	7.524×10^{-3}	4.455×10^{-4}
$\tau = 10^{-5}$	$t = 10000\tau$	$t = 20000\tau$	$t = 50000\tau$	$t = 100000\tau$
A.E.	7.884×10^{-6}	2.686×10^{-5}	2.831×10^{-5}	5.012×10^{-5}
P.E.	1.447×10^{-3}	3.031×10^{-3}	5.368×10^{-3}	5.784×10^{-3}

From the results of table 1 we can see that the method is of high accuracy.

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