



An efficient block Gauss–Seidel iteration method for the space fractional coupled nonlinear Schrödinger equations



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ABSTRACT

In this paper, we propose an efficient block Gauss–Seidel iteration method for solving the complex linear equations arising from the space fractional coupled nonlinear Schrödinger (CNLS) equations. The proposed method avoids the inverse of coefficient matrix when solving linear equations, which can greatly reduce computation load and storage space. Furthermore, the convergence of the iteration method is proved theoretically and the number of iteration steps is estimated. Numerical results are presented to show the block Gauss–Seidel iteration method can be quite competitive when compared with others.

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1. Introduction

The Schrödinger equations are the basic equation of quantum mechanics. They describe nonrelativistic quantum mechanical behaviors, and they can be derived from the path integral over the Brownian motion. A fractional generalization of the Schrödinger equation has been found by extending the Brownian motion to the Lévy- α process [1]. In this work, we consider the space fractional coupled nonlinear Schrödinger (CNLS) equations

$$\begin{cases} iu_t + \gamma(-\Delta)^{\frac{\alpha}{2}}u + \rho(|u|^2 + \beta|v|^2)u = 0, \\ iv_t + \gamma(-\Delta)^{\frac{\alpha}{2}}v + \rho(|v|^2 + \beta|u|^2)v = 0, \end{cases} \quad a \leq x \leq b, \quad 0 < t \leq T \quad (1.1)$$

with the initial boundary value conditions $u(x, 0) = u_0(x)$, $v(x, 0) = v_0(x)$, $u(a, t) = u(b, t) = 0$ and $v(a, t) = v(b, t) = 0$, where $i = \sqrt{-1}$, $1 < \alpha < 2$ and the parameters $\gamma, \rho > 0$, $\beta \geq 0$ are some constants. The fractional Laplacian [2] operator in (1.1) can be characterized as $(-\Delta)^{\frac{\alpha}{2}}u(x, t) = \mathcal{F}^{-1}(|\xi|^\alpha \mathcal{F}(u(x, t)))$,

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where \mathcal{F} is the Fourier transform acting on the spatial variable x . The Riesz fractional derivative [3] can also be defined as

$$\frac{\partial^\alpha}{\partial|x|^\alpha}u(x,t) = -(-\Delta)^{\frac{\alpha}{2}}u(x,t) = -\frac{1}{2\cos\frac{\pi\alpha}{2}}[-_\infty D_x^\alpha u(x,t) + {}_x D_{+\infty}^\alpha u(x,t)], \tag{1.2}$$

where ${}_{-\infty}D_x^\alpha u(x,t)$ and ${}_x D_{+\infty}^\alpha u(x,t)$ are the left and right Riemann–Liouville fractional derivatives, respectively. The left and right Riemann–Liouville fractional derivatives of order α are defined as

$$\begin{aligned} {}_{-\infty}D_x^\alpha u(x,t) &= \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_{-\infty}^x(x-\tau)^{n-1-\alpha}u(\tau,t)d\tau, \\ {}_x D_{+\infty}^\alpha u(x,t) &= \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_x^{+\infty}(\tau-x)^{n-1-\alpha}u(\tau,t)d\tau. \end{aligned} \tag{1.3}$$

However, the nonlocal nature of the fractional operator often leads to the inability to obtain the exact solution of fractional differential equations. Hence, numerical methods become an important tool to understand the behavior of fractional differential equations. Recently, a number of numerical methods are developed for discretizing the nonlinear Schrödinger equations. For example, the difference methods for the space fractional coupled nonlinear Schrödinger equations (CNLS) are studied in [4–6]. In [7] authors solved the space fractional Schrödinger equation numerically via the Crank–Nicholson scheme.

The coefficient matrix of the discretized linear system is equal to the sum of a complex scaled identity matrix, a diagonal matrix and a symmetric Toeplitz matrix. In recent years, Ran et al. [8,9] proposed the partially inexact HSS iteration method and HSS-like iteration method for the discretized linear system motivated by the Hermitian and skew-Hermitian splitting (HSS) method [10]. Wang [11] presented the preconditioned modified Hermitian and skew-Hermitian splitting (PMHSS) iteration method and gave the unconditional convergent theoretical analysis.

In this paper, we construct the proper two-by-two linear system and apply block Gauss–Seidel iteration method to solve the corresponding linear systems without solving the inverse of the coefficient matrices, which can greatly reduce the computation cost and accelerate the computing speed. Meanwhile, the block Gauss–Seidel iteration method does not need to adjust the parameters, and is independently of parameters, and we analyze the spectral property of the iteration matrix and prove the convergence theory of the block Gauss–Seidel iteration method.

The paper is organized as follows. Section 2 refers to the discretization of the space fractional CNLS equations. In Section 3 we apply the block Gauss–Seidel iteration method to solve the two-by-two linear system and establish its convergence theory. In Section 4, numerical examples are given.

2. Discretization of the space fractional CNLS equations

Let M and N be given positive integers, $\tau = T/N$ and $h = (b - a)/(M + 1)$. Define $t_n := n\tau$ for $n = 0, 1, \dots, N$ and $x_j := a + jh$ for $j = 0, 1, \dots, M + 1$. And u_j^n and v_j^n denote the numerical approximations to $u(x_j, t_n)$ and $v(x_j, t_n)$. The fractional Laplacian $(-\Delta)^{\frac{\alpha}{2}}$ is discretized by the fractional centered difference [12] in the truncated bounded domain as

$$(-\Delta)^{\frac{\alpha}{2}}u(x_j) = -\frac{\partial^\alpha}{\partial|x|^\alpha}u(x_j) = \frac{1}{h^\alpha}\sum_{k=1}^M c_{j-k}u_k + \mathcal{O}(h^2),$$

where the coefficients $c_k = \frac{(-1)^k \Gamma(\alpha+1)}{\Gamma(\alpha/2-k+1)\Gamma(\alpha/2+k+1)}$, with $\tau(\cdot)$ being the gamma function. The coefficients c_k satisfy the following properties

$$c_0 \geq 0, \quad c_k = c_{-k} \leq 0, \quad k = 1, 2, \quad \sum_{k=-\infty, k \neq 0}^{+\infty} |c_k| = c_0. \tag{2.1}$$

Using the linearly implicit difference scheme proposed in [4], we obtain the following linearly implicit difference scheme for the model (1.1)

$$\begin{cases} i \frac{u_j^{n+1} - u_j^{n-1}}{2\tau} + \frac{\gamma}{h^\alpha} \sum_{k=1}^M c_{j-k} \left(\frac{u_k^{n+1} + u_k^{n-1}}{2} \right) + \rho \left(|u_j^n|^2 + \beta |v_j^n|^2 \right) \frac{u_j^{n+1} + u_j^{n-1}}{2} = 0, \\ i \frac{v_j^{n+1} - v_j^{n-1}}{2\tau} + \frac{\gamma}{h^\alpha} \sum_{k=1}^M c_{j-k} \left(\frac{v_k^{n+1} + v_k^{n-1}}{2} \right) + \rho \left(|v_j^n|^2 + \beta |u_j^n|^2 \right) \frac{v_j^{n+1} + v_j^{n-1}}{2} = 0, \end{cases} \quad (2.2)$$

where $j = 1, 2, \dots, M, n = 1, 2, \dots, N - 1$, and in [4,5] the authors proved that the scheme (2.2) conserves the discrete mass and energy, and is unconditionally stable and converges with order $\mathcal{O}(\tau^2 + h^2)$ in the discrete l_2 norm. According to the initial boundary value conditions, we have $u_j^0 = u_0(x_j), v_j^0 = v_0(x_j), u_0^n = u_{M+1}^n = 0, v_0^n = v_{M+1}^n = 0$. Also, the first step can be proposed by some second or higher order temporal integrators. In (2.2), the first and the second difference equations have the same structure. Denote $u^{n+1} = [u_1^{n+1}, \dots, u_M^{n+1}]^T, b^{n+1} = [b_1^{n+1}, \dots, b_M^{n+1}]^T, \mu = \frac{\gamma\tau}{h^\alpha}, d_j^{n+1} = \rho\tau \left(|u_j^n|^2 + \beta |v_j^n|^2 \right)$, where

$$b_j^{n+1} = iu_j^{n-1} - \mu \sum_{k=1}^M c_{j-k} u_k^{n-1} - d_j^{n+1} u_j^{n-1}, j = 1, 2, \dots, M.$$

If we further denote $D^{n+1} = \text{diag}(d_1^{n+1}, d_2^{n+1}, \dots, d_M^{n+1})$ and I is the identity matrix, then the first difference scheme in (2.2) can be rewritten as

$$A^{n+1} u^{n+1} = b^{n+1}, n = 1, 2, \dots, N - 1 \quad (2.3)$$

where the coefficient matrix A^{n+1} is composed by $A^{n+1} = iI + D^{n+1} + T$. Here, T is the Toeplitz matrix

$$T = \mu \begin{pmatrix} c_0 & c_{-1} & \cdots & c_{2-M} & c_{1-M} \\ c_1 & c_0 & \cdots & c_{3-M} & c_{2-M} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{M-2} & c_{M-3} & \cdots & c_0 & c_{-1} \\ c_{M-1} & c_{M-2} & \cdots & c_1 & c_0 \end{pmatrix}. \quad (2.4)$$

According to the parameters $\gamma, \rho > 0, \beta \geq 0$ and the properties of the coefficient c_k , we can get that the Toeplitz matrix T is strictly diagonally dominant and symmetric positive definite, and D^{n+1} is a nonnegative diagonal matrix. Therefore, the matrix $D^{n+1} + T$ is symmetric positive definite. Based on the above properties, then the matrix A^{n+1} is complex symmetric and non-Hermitian positive definite.

3. Block Gauss–Seidel iteration method

In this section, we apply the block Gauss–Seidel iteration method to solve the linear system (2.2) and establish its convergence theory. Furthermore, the corresponding iteration steps of the iteration method are estimated.

We consider the following complex linear equation

$$Au = b, \quad A \in \mathbb{C}^{M \times M} \text{ nonsingular, and } u, b \in \mathbb{C}^M, \quad (3.1)$$

where $A = D + T + iI$ is a complex symmetric matrix with $i = \sqrt{-1}$ is the imaginary unit, I is the identity matrix, $D = \text{diag}(d_1, d_2, \dots, d_M)$ is the nonnegative diagonal matrix and T is the symmetric positive definite

Toeplitz matrix defined in (2.4). Here $u = y + iz$ and $b = p + iq$ are complex vectors with y, z, p, q are real vectors in \mathbb{R}^M . However, the matrix A contains complex value and the matrix T is a full matrix with Toeplitz structure. Therefore, the workload will be heavy if HSS-based iteration methods are used. In this paper, by transforming the complex linear system into the two by-two linear system and utilizing the block Gauss–Seidel iteration method, we will construct a new fast iterative method for solving the system of complex linear equations (3.1). The new method will avoid complex value arithmetics and computing the matrix inverse. The complex linear system (3.1) is equivalent to a two-by-two linear system as

$$Mx \equiv \begin{pmatrix} -I & W \\ W & I \end{pmatrix} \begin{pmatrix} z \\ y \end{pmatrix} = \begin{pmatrix} p \\ q \end{pmatrix} \equiv g, \tag{3.2}$$

where $W = D + T$. Then we develop the block Gauss–Seidel iterative method [13] for (3.2) as follows:

Block Gauss–Seidel iteration method. Given an initial guess $(y^{(0)T}, z^{(0)T}) \in \mathbb{R}^{2M}$, for $k = 0, 1, 2, \dots$, until the iteration sequence $\{(y^{(k)T}, z^{(k)T})\}_{k=0}^\infty \in \mathbb{R}^{2M}$ converges, compute the next iterate $(y^{(k+1)T}, z^{(k+1)T})$ according to the following procedure:

$$\begin{cases} -I \cdot z^{(k+1)} = p - W \cdot y^{(k)}, \\ I \cdot y^{(k+1)} = q - W \cdot z^{(k+1)}. \end{cases} \tag{3.3}$$

According to the above equation (3.3), we can observe that the coefficient matrices are both identity matrices, hence solving the inverse of matrix does not need to be involved in the iteration process, which greatly reduces the computational load and memory requirement. Therefore, when using the block Gauss–Seidel iteration method to solve linear system (3.1), the main computing cost per iteration of the block Gauss–Seidel iteration method comes from the matrix–vector multiplication. Meanwhile, we observe that W is composed of diagonal matrix and Toeplitz matrix, so we can use fast Fourier method to calculate matrix–vector multiplication, which greatly reduces the amount of calculation. The sequence in (3.3) could be reformulated as

$$y^{(k+1)} = -W^2 \cdot y^{(k)} + W \cdot p + q \tag{3.4}$$

where $L := -W^2$ is the corresponding iteration matrix. For the convergence property of the block Gauss–Seidel iteration method, we have the following result. Here and in the sequel, we use $\|\cdot\|_2$ to denote the Euclidean norm and $\|\cdot\|_\infty$ to denote the infinite norm. Before proving the convergence of the block Gauss–Seidel iteration method, we first give the relevant lemma.

Lemma 3.1 ([4,5]). *For the difference scheme (2.2), there exists a unique bounded solution.*

Then we prove that the block Gauss–Seidel iteration method converges by the following theorem.

Theorem 3.1. *Let A be a complex symmetric matrix defined as in (3.1) with D and T being positive diagonal matrix and symmetric positive definite Toeplitz matrix respectively. The iteration matrix L is given by $L = -(D + T)^2$, and define the parameters $\rho, C > 0, \beta \geq 0$ are some constants. Then, the following estimate of the spectral radius $\rho(L)$ of the iteration matrix L holds*

$$\rho(L) < 1,$$

and the iteration sequence $\{(y^{(k)T}, z^{(k)T})\}_{k=0}^\infty$, yielded by the block Gauss–Seidel iteration method starting from any initial vector $(y^{(0)T}, z^{(0)T}) \in \mathbb{R}^{2M}$, converges to the unique solution of the discrete linear system in Eq. (3.1), provided that the time step τ and space step h satisfy the condition

$$\sigma\tau + 3\mu c_0 < 1.$$

Proof. Let $d = \max\{d_j\}$ and $\hat{d} = \min\{d_j\}$, by the Geršgorin disk theorem [14] that all eigenvalues of A must belong to the union of n disks as follows $G(\mathbf{A}) = \bigcup_{i=1}^n \left\{ z \in \mathbb{C} \mid |z - a_{ii}| \leq R_i(\mathbf{A}) = \sum_{j=1, j \neq i}^n |a_{ij}| \right\}$. Thus, we can obtain the estimation of the eigenvalue range of the matrix W as follows

$$|\lambda - (d_j + \mu c_0)| < 2\mu \sum_{i=1}^{M-1} |c_i|,$$

which leads to

$$d_j + \mu c_0 - 2\mu \sum_{i=1}^{M-1} |c_i| < \lambda < d_j + \mu c_0 + 2\mu \sum_{i=1}^{M-1} |c_i|,$$

according to the properties of (2.1), we have

$$\hat{d} - \mu c_0 < \lambda < d + 3\mu c_0.$$

According to Lemma 3.1 that for the discrete scheme (2.2), there exists a unique bounded solution, so we have

$$\|u^n\|_\infty \leq C, \quad \|v^n\|_\infty \leq C, \tag{3.5}$$

where C is a constant, then

$$\begin{aligned} & d + 3\mu c_0 \\ &= \max\{\rho\tau \left(|u_j^n|^2 + \beta |v_j^n|^2 \right)\} + 3\mu c_0 \\ &\leq \rho\tau(1 + \beta)|C|^2 + 3\mu c_0 \\ &= \sigma\tau + 3\mu c_0, \end{aligned}$$

where $\sigma = \rho(1 + \beta)|C|^2$. From the above derivation, we can also obtain the range of infinite norm of W

$$\|W\|_\infty < \sigma\tau + 3\mu c_0. \tag{3.6}$$

By observing Eq. (3.6), we can see that σ and c_0 are constants, then the numerical range of formula (3.6) can be controlled by appropriate τ and h . Therefore, we can select appropriate τ and h to make the formula (3.6) less than 1. By norm consistency principle, we have

$$\rho(L) \leq \|W^2\|_\infty \leq \|W\|_\infty \|W\|_\infty < 1 \tag{3.7}$$

which finishes the proof. \square

Next, we obtain an estimate of the iteration steps of the block Gauss–Seidel iteration method.

Theorem 3.2. Let $e^{(k+1)} = y^{(k+1)} - y_*$ with y_* is the exact solution, according to the iterative scheme (3.4), the following l_∞ estimate of iteration step k holds

$$k > \log_\delta c,$$

where ϵ , δ and c are constants.

Proof. According to (3.4)

$$y^{(k+1)} = -W^2 y^{(k)} + Wp + q,$$

we have $e^{(k+1)} = -W^2 e^{(k)}$. Then the following relation holds

$$\|e^{(k+1)}\|_\infty \leq \|W^2\|_\infty \|e^{(k)}\|_\infty \leq \|W\|_\infty^{2k} \|e^{(1)}\|_\infty.$$

On the basis of the (3.7), we know that $\|W\|_\infty$ is bounded and less than 1, and $\|e^{(1)}\|_\infty$ is a constant, we could suppose $\|e^{(k+1)}\|_\infty \leq \|W\|_\infty^{2k} \|e^{(1)}\|_\infty < \epsilon$, which leads to

$$\|W\|_\infty^{2k} < \frac{\epsilon}{\|e^{(1)}\|_\infty}. \tag{3.8}$$

Denote $c = \frac{\epsilon}{\|e^{(1)}\|_\infty}$, and according to Theorem 3.1, we can make $\|W\|_\infty^2 < \delta$. If we take logarithms on both sides of the inequality (3.8), then we have

$$k > \frac{\log c}{\log \|W\|_\infty^2},$$

which leads to

$$k > \log_\delta c,$$

which finishes the proof. \square

4. Numerical experiments

In this section, we give two numerical experiments to test the performance of the proposed block Gauss–Seidel iteration method (denote by BG-S) to solve the linear systems arising from two fractional nonlinear Schrödinger equations. The GMRES method tested here is restarted version with a restarting number 40. We will also present the performance of the preconditioned modified Hermitian and skew-Hermitian splitting iteration methods (PMHSS) developed in [11]. Denote by PIHSS the partially inexact HSS iteration methods in [8]. Also, denote by HSS-like the HSS-like iteration method proposed by [9]. All numerical experiments are performed via MATLAB R2018b on a PC. All parameters are set to be the experimentally optimal parameter. All numerical experiments are started from the zero vector, and terminated when the current iterate satisfies $\frac{\|r_k\|_2}{\|r_0\|} < 10^{-6}$, where r_k is the residual vector of the k th iteration and r_0 is the initial residual vector.

Experiment 1. Let $\gamma = 1, \rho = 2, \beta = 0, 1 < \alpha < 2$. Then the system (1.1) is decoupled and becomes

$$iu_t + (-\Delta)^{\frac{\alpha}{2}} u + 2|u|^2 u = 0, \quad -20 \leq x \leq 20, \quad 0 < t \leq 2, \tag{4.1}$$

subjected to the initial boundary value conditions $u(x, 0) = \text{sech}(x) \cdot \exp(2ix), u(-20, t) = u(20, t) = 0$.

Experiment 2. For the following coupled system with $\gamma = 1, \rho = 2, \beta = 1, 1 < \alpha < 2$,

$$\begin{cases} iu_t + (-\Delta)^{\frac{\alpha}{2}} u + 2(|u|^2 + |v|^2) u = 0, \\ iv_t + (-\Delta)^{\frac{\alpha}{2}} v + 2(|v|^2 + |u|^2) v = 0, \end{cases} \quad -20 \leq x \leq 20, \quad 0 < t \leq 2, \tag{4.2}$$

we take the initial boundary value conditions in the form

$$\begin{cases} u(x, 0) = \text{sech}(x + 1) \cdot \exp(2ix), v(x, 0) = \text{sech}(x - 1) \cdot \exp(-2ix), \\ u(-20, t) = u(20, t) = 0, v(-20, t) = v(20, t) = 0. \end{cases} \tag{4.3}$$

The numerical results are listed in Tables 1–4. We denote the number of spatial grid points by M , the number of iterations of the methods by “Iter” and the computational time of solving the whole discrete system by “CPU”. Here, α is the order of the spatial fractional equations. From these tables, it is clear that the computation time of the block Gauss–Seidel iteration method is obviously the least. At the same time, the number of iteration steps of the block Gauss–Seidel iteration method is the smallest, and there

Table 1

CPU times and the number of iterations for BG-S, PMHSS, PIHSS, HSS-like and GMRES(40) with $\alpha = 1.2$ and $N = 4M$ for Experiment 1.

M	800		1600		3200		6400	
	Iter	CPU (s)						
BG-S	2	2.20e-3	2	1.16e-2	2	3.47e-2	2	1.59e-1
PMHSS	40	1.97	40	16.45	40	85.80	40	439.29
Gmres(40)	4	5.50e-3	4	1.75e-2	4	6.11e-2	4	2.25e-1
PIHSS	77	18.21	104	92.38	111	395.99	110	1.54e+3
HSS-like	154	37.01	162	141.63	150	518.35	136	1.85e+3

Table 2

CPU times and the number of iterations for BG-S, PMHSS, PIHSS, HSS-like and GMRES(40) with $\alpha = 1.7$ and $N = 6M$ for Experiment 1.

M	800		1600		3200		6400	
	Iter	CPU (s)						
BG-S	2	2.20e-3	2	1.11e-2	2	4.35e-2	5	3.52e-1
PMHSS	40	1.15	40	6.25	40	28.32	40	166.33
GMRES(40)	4	5.30e-3	5	1.90e-2	6	8.28e-2	7	3.73e-1
PIHSS	247	111.61	385	823.83	413	4.13e+3	689	3.54e+4
HSS-like	418	285.63	435	1.43e+3	539	8.55e+3	1395	1.17e+5

Table 3

CPU times and the number of iterations for BG-S, PMHSS, PIHSS, HSS-like and GMRES(40) with $\alpha = 1.2$ and $N = 6M$ for Experiment 2.

M	800		1600		3200		6400	
	Iter	CPU (s)						
BG-S	4	3.7e-3	4	1.91e-2	4	7.97e-2	4	2.89e-1
PMHSS	80	2.32	80	11.75	80	59.53	80	325.84
GMRES(40)	8	2.59e-2	8	3.52e-2	8	1.17e-1	8	4.84e-1
PIHSS	199	36.34	289	188.01	314	8.08e+2	313	3.40e+3
HSS-like	232	59.25	244	222.59	227	8.11e+2	229	3.45e+3

is no obvious increase. We also figure that the block Gauss–Seidel iteration method can achieve the same computation effect as the GMRES method, and more often, the computation effect of the block Gauss–Seidel iteration method is better than that of the GMRES method. For instance, in Table 3, when $M = 800$, the computation time of GMRES is seven times that of the block Gauss–Seidel iteration method, and the number of iteration steps is also two times. Meanwhile, we can see that the computation time of PMHSS, PIHSS and HSS-like is much longer than that of the block Gauss–Seidel iteration method, and their iteration steps are very large and have been increasing. Thus, the BG-S method outperforms PMHSS, Gmres, PIHSS and HSS-like methods considerably in terms of the number of iterations and CPU time.

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Table 4

CPU times and the number of iterations for BG-S, PMHSS, PIHSS, HSS-like and GMRES(40) with $\alpha = 1.7$ and $N = 8M$ for Experiment 2.

M	800		1600		3200		6400	
	Iter	CPU (s)						
BG-S	4	9.40e-3	4	1.93e-2	4	8.08e-2	13	9.71e-1
PMHSS	80	2.32	80	11.26	80	57.74	80	309.10
GMRES(40)	8	2.43e-2	8	3.72e-2	8	1.42e-1	14	7.88e-1
PIHSS	430	192.68	697	1.41e+3	778	7.77e+3	1404	7.47e+4
HSS-like	505	463.26	591	2.60e+3	1812	4.16e+4	-	-

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