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On partially inexact HSS iteration methods for the complex symmetric linear systems in space fractional CNLS equations

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Abstract

The space fractional coupled nonlinear Schrödinger (CNLS) equations are discretized by an implicit conservative difference scheme with the fractional centered difference formula, which is unconditionally stable. The coefficient matrix of the discretized linear system is equal to the sum of a complex scaled identity matrix and a symmetric positive definite diagonal-plus-Toeplitz matrix. The Hermitian and skew-Hermitian splitting (HSS) method and the partially inexact HSS (PIHSS) method are employed to solve the discretized linear system. In the inner iteration processes of the HSS method, we only need to solve the linear sub-systems associated with the Hermitian part inexactly by the conjugate gradient (CG) method, resulting in PIHSS iteration method. Theoretical analyses show that both HSS and PIHSS methods are unconditionally convergent. Numerical examples are given to demonstrate the effectiveness of the HSS iteration and the PIHSS iteration.

Keywords: The space fractional Schrödinger equations; Hermitian and skew-Hermitian splitting; Inexact iterations; Conjugate gradient method; Convergence analysis

1 Introduction

In this paper, we consider the space fractional coupled nonlinear Schrödinger (CNLS) equations

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

with the initial boundary value conditions

$$\begin{cases} u(x,0) = u_0(x), & v(x,0) = v_0(x), & a \le x \le b, \\ u(a,t) = u(b,t) = 0, & v(a,t) = v(b,t) = 0, & 0 \le t \le T, \end{cases}$$

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where $i = \sqrt{-1}$, $1 < \alpha < 2$ and the parameters $\gamma > 0$, $\rho > 0$, $\beta \geq 0$ are constants. The fractional Laplacian [9] can be characterized as

$$(-\Delta)^{\frac{\alpha}{2}} u(x,t) = \mathcal{F}^{-1}\Big(|\xi|^{\alpha}\mathcal{F}(u(x,t))\Big),$$

where $\mathcal{F}$ is the Fourier transform acting on the spatial variable x. Furthermore, it is shown that the Riesz fractional derivative [21] can also be defined as

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

where ${}_{-\infty}D_x^{\alpha}u(x,t)$ and ${}_xD_{+\infty}^{\alpha}u(x,t)$ are the left and right Riemann-Liouville derivatives, respectively.

The classical Schrödinger equations describe the evolution of microscopic particles, and they can be derived from the path integral over the Brownian motion. Laskin [12] generalized the path integral method from the Brownian motion to the Lévy-α process to obtain the space fractional Schrödinger equations. Many papers focus on the solution of the fractional Schrödinger equations. Generally, it is very difficult to obtain the exact solutions of fractional differential equations because of the nonlocal nature of the fractional operator. Consequently, the numerical methods become important and powerful tools to understand the behaviors of fractional differential equations [1, 2, 11]. But for the fractional Schrödinger equations, the numerical methods are very few until now.

The main problem for the numerical methods for the space fractional CNLS equations is to discretize the fractional Laplacian operator. Because of the nonlocal property of fractional differential operator, a simple discretization scheme of the space fractional CNLS equations, even though implicit, lead to be unconditionally unstable and lead to dense or full matrices. In order to reduce the computation complexity and memory requirement, Ortigueira [16] proposed the so-called fractional centered difference to approximate the fractional Laplacian operator. This method is of the second-order accuracy. Furthermore, the full coefficient matrix by the Ortigueira's method holds special complex symmetric structure, which can be written as the sum of the complex scaled identity matrix and the symmetric positive definite diagonal-plus-Toeplitz matrix [18–20].

As the resulting discretized systems are the complex symmetric linear systems, Bai et al. [5] presented the Hermitian and skew-Hermitian splitting (HSS) iteration and the inexact HSS (IHSS) iteration which employs some Krylov subspace methods as its inner iteration processes at each step of the outer HSS iteration to compute an approximate solution for non-Hermitian positive definite linear systems. There is now considerable evidence that the good convergence properties of the HSS iteration method are preserved even when the inner solves are performed to rather low accuracy, resulting in significant savings, especially for very large problems. A potential difficulty with the HSS iteration approach is need to solve the shifted skew-Hermitian sub-systems at each iteration step. However, the Krylov subspace iterations need to be implemented in complex arithmetic. Moreover, their convergence rates tend to be considerably worse. In order to overcome the disadvantage of the HSS method, Bai et al. [3] proposed the modified HSS iteration method for the complex symmetric linear systems. A considerable advantage of the modified HSS iteration consists in the fact that it is unnecessary to solve the linear sub-system associated with the skew-Hermitian part and only two symmetric positive definite linear sub-systems need to be solved at each step. To further generalized the modified HSS iteration method and accelerate its convergence rate, the preconditioned modified HSS iteration method is proposed in [4].

The main aim of this paper is to solve the complex symmetric linear systems from the discretization of the space fractional CNLS equations. The coefficient matrix of the discretized linear system is equal to the sum of the complex scaled identity matrix and the symmetric positive definite diagonal-plus-Toeplitz

matrix. The HSS and the partially inexact HSS (PIHSS) methods [6] are applied to solve the discretized linear system. At each HSS iteration step, we only need to solve the linear sub-system associated with the Hermitian part inexactly by the conjugate gradient (CG) method [10]. This may result in PIHSS iteration method.

The remaining of the paper is outlined as follows. In Section 2, we present the discretized system. In Section 3, we employ the HSS method and the PIHSS method to solve the discretized system, and study their convergence properties. In Section 4, numerical examples are given to show the effectiveness of the HSS method and the PIHSS method. Finally, concluding remarks are presented in Section 5.

2 Discretization of the space fractional CNLS equations

Let $\tau = T/N$ and $h = (b-a)/(M+1)$ be the sizes of time step and spatial grid, respectively, where N and M are positive integers. We define a temporal and spatial partition $t_n = n\tau$ for $n = 0, 1, \ldots, N$ and $x_j = a + jh$ for $j = 0, 1, \ldots, M+1$. Let $u_j^n \approx u(x_j, t_n)$ and $v_j^n \approx v(x_j, t_n)$ denote the corresponding numerical solutions. By the fractional centered difference [16], we can discrete the fractional Laplacian $(-\Delta)^{\frac{\alpha}{2}}$ in the truncated bounded domain as

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

where the coefficients

$$c_k = \frac{(-1)^k \Gamma(\alpha+1)}{\Gamma(\alpha/2-k+1)\Gamma(\alpha/2+k+1)},$$

with $\Gamma(\cdot)$ being the gamma function. Moreover, the coefficients c_k satisfy the following properties

$$\begin{cases} c_0 \geq 0, \\ c_k = c_{-k} \leq 0, \quad k = 1, 2, \ldots, \\ \sum\limits_{k=-\infty, k\neq 0}^{+\infty} |c_k| = c_0. \end{cases}$$

They proposed the following implicit difference scheme for the space fractional CNLS equations (1.1)

$$\begin{cases} i\frac{u_j^{n+1}-u_j^{n-1}}{2\tau} + \frac{\gamma}{h^\alpha} \sum\limits_{k=1}^{M} c_{j-k}\Big(\frac{u_k^{n+1}+u_k^{n-1}}{2}\Big) + \rho\Big(|u_j^n|^2 + \beta|v_j^n|^2\Big)\frac{u_j^{n+1}+u_j^{n-1}}{2} = 0, \\ i\frac{v_j^{n+1}-v_j^{n-1}}{2\tau} + \frac{\gamma}{h^\alpha} \sum\limits_{k=1}^{M} c_{j-k}\Big(\frac{v_k^{n+1}+v_k^{n-1}}{2}\Big) + \rho\Big(|v_j^n|^2 + \beta|u_j^n|^2\Big)\frac{v_j^{n+1}+v_j^{n-1}}{2} = 0, \end{cases} \tag{2.1}$$

where $j = 1, 2, \ldots, M, n = 1, 2, \ldots, N-1$, and proved that the scheme (2.1) is unconditionally stable [18–20]. By the initial boundary value conditions, we have

$$u_j^0 = u_0(x_j), \quad v_j^0 = v_0(x_j), \quad u_0^n = u_{M+1}^n = 0, \quad v_0^n = v_{M+1}^n = 0.$$

In addition, the first step can be obtained by some second or higher order time integrators. The structure of the first difference equation in (2.1) is the same as the second one. Denote

$$u^{n+1} = \Big[u_1^{n+1}, \ldots, u_M^{n+1}\Big]^T, \; b^{n+1} = \Big[b_1^{n+1}, \ldots, b_M^{n+1}\Big]^T, \; \eta = \frac{1}{2\tau}, \; \mu = \frac{\gamma}{2h^\alpha}, \; d_j^{n+1} = \frac{\rho}{2}\Big(|u_j^n|^2 + \beta|v_j^n|^2\Big),$$

where

$$b_j^{n+1} = i\eta u_j^{n-1} - \mu \sum_{k=1}^{M} c_{j-k} u_k^{n-1} - d_j^{n+1} u_j^{n-1}, \quad j = 1, 2, \ldots, M.$$

Then we can rewrite the first difference scheme in (2.1) into the following matrix vector form

$$A^{n+1} u^{n+1} = b^{n+1}, \quad n = 1, 2, \ldots, N-1, \tag{2.2}$$

where the coefficient matrix A^{n+1} is of the form

$$A^{n+1} = i\eta I + D^{n+1} + T.$$

Here I is the identity matrix, D^{n+1} is the diagonal matrix defined by $D^{n+1} = \mathrm{diag}(d_1^{n+1}, d_2^{n+1}, \ldots, d_M^{n+1})$ and T is the Toeplitz matrix

$$T = \mu \begin{pmatrix} c_0 & c_{-1} & \cdots & c_{2-M} & c_{1-M} \\ c_1 & c_0 & \cdots & c_{3-M} & c_{2-M} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{M-2} & c_{M-3} & \cdots & c_0 & c_{-1} \\ c_{M-1} & c_{M-2} & \cdots & c_1 & c_0 \end{pmatrix}. \tag{2.3}$$

From the fact $\gamma > 0$, $\rho > 0$, $\beta \geq 0$ and the properties of the coefficients c_k we see that the Toeplitz matrix T is symmetric strictly diagonally dominant, then symmetric positive definite, and D^{n+1} is non-negative diagonal matrix. Thus, the matrix $D^{n+1} + T$ is symmetric positive definite. Based on these facts, the coefficient matrix A^{n+1} is complex symmetric and non-Hermitian positive definite.

3 The PIHSS iteration method

In the following, we consider the iterative solution of the system of linear equations

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

where A is a complex symmetric matrix of the form

$$A = D + T + i\eta I \tag{3.2}$$

and $\eta > 0$, $i = \sqrt{-1}$ is the imaginary unit, I is the identity matrix, $D = \mathrm{diag}(d_1, \ldots, d_M)$ is the nonnegative diagonal matrix with $d_i \geq 0, i = 1, \ldots, M$, T is the symmetric positive definite Toeplitz matrix defined in (2.3).

The Hermitian and skew-Hermitian parts of the matrix A in (3.2) are given by

$$H = \frac{A + A^*}{2} = \frac{(D + T + i\eta I) + (D + T + i\eta I)^*}{2} = D + T,$$

and

$$S = \frac{A - A^*}{2} = \frac{(D + T + i\eta I) - (D + T + i\eta I)^*}{2} = i\eta I,$$

respectively, here A^* is the conjugate transpose of the matrix A. Obviously, the Hermitian part H is symmetric positive definite. Then A is the non-Hermitian but positive definite matrix. Thus, we can

straightly employ the HSS iteration method to compute an approximate solution of the non-Hermitian positive definite linear system (3.1), and it is as follows.

The HSS iteration method for the linear system (3.1). Given an initial guess $u^{(0)}$, for $k = 0, 1, 2, \ldots$, until $\{u^{(k)}\}$ converges, compute

$$\begin{cases} (\tilde{\alpha}I + D + T)u^{(k+\frac{1}{2})} = (\tilde{\alpha} - i\eta)u^{(k)} + b, \\ u^{(k+1)} = \frac{1}{\tilde{\alpha}+i\eta}[(\tilde{\alpha}I - D - T)u^{(k+\frac{1}{2})} + b], \end{cases}$$

where $\tilde{\alpha}$ is a given positive constant and I is the identity matrix.

The iteration matrix $M(\tilde{\alpha})$ of the HSS iteration method for the linear system (3.1) is given by

$$M(\tilde{\alpha}) = \frac{\tilde{\alpha} - i\eta}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\tilde{\alpha}I + D + T)^{-1},$$

and its spectral radius $\rho(\tilde{\alpha})$ is

$$\rho(\tilde{\alpha}) = \max_{\lambda_i \in \lambda(D+T)} \left|\frac{\tilde{\alpha} - \lambda_i}{\tilde{\alpha} + \lambda_i}\right|,$$

where $\lambda(D + T)$ is the spectral set of the symmetric positive definite matrix $D + T$. Since $\lambda_i > 0$ for $\forall \lambda_i \in \lambda(D + T)$, it holds that

$$\rho(\tilde{\alpha}) < 1, \quad \forall \tilde{\alpha} > 0.$$

Thus, the HSS iteration method converges to the unique solution of the system of linear equations (3.1).

Moreover, if λ_1 and λ_M are the minimum and the maximum eigenvalues of the matrix $D + T$, respectively, then the optimal parameter $\tilde{\alpha}^*$ is

$$\tilde{\alpha}^* = \sqrt{\lambda_1 \lambda_M} \quad \text{and} \quad \rho(\tilde{\alpha}^*) = \frac{\sqrt{\lambda_M} - \sqrt{\lambda_1}}{\sqrt{\lambda_M} + \sqrt{\lambda_1}} = \frac{\sqrt{\kappa_h} - 1}{\sqrt{\kappa_h} + 1},$$

where $\kappa_h = \frac{\lambda_M}{\lambda_1}$ is the spectral condition number of $D + T$. We emphasize that, the optimal parameter $\tilde{\alpha}^*$ minimizes the spectral radius $\rho(\tilde{\alpha})$ itself and thus is really the optimal parameter in theory.

The 2-norms of the matrices $(\tilde{\alpha} - i\eta)(\tilde{\alpha}I + D + T)^{-1}$ and $\frac{1}{\tilde{\alpha}+i\eta}(\tilde{\alpha}I - D - T)$ are given in the following theorem which will be useful later.

Theorem 3.1. *Let $A \in \mathbb{C}^{M\times M}$ be defined in (3.2), $D + T$ and $i\eta I$ be its Hermitian and skew-Hermitian parts, respectively, and $\tilde{\alpha}$ be a positive constant. Then*

$$c_h(\tilde{\alpha}) \equiv \|(\tilde{\alpha} - i\eta)(\tilde{\alpha}I + D + T)^{-1}\|_2 = \frac{\sqrt{\tilde{\alpha}^2 + \eta^2}}{\tilde{\alpha} + \lambda_1},$$
$$c_s(\tilde{\alpha}) \equiv \|\frac{1}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)\|_2 = \frac{1}{\sqrt{\tilde{\alpha}^2 + \eta^2}} \max\left\{|\tilde{\alpha} - \lambda_1|, |\tilde{\alpha} - \lambda_M|\right\}.$$

In particular, when $\tilde{\alpha} = \tilde{\alpha}^* = \sqrt{\lambda_1 \lambda_M}$, and let $\kappa_{h,s} = 1 + \frac{\eta^2}{\lambda_1 \lambda_M}$, then it holds that

$$c_h(\tilde{\alpha}^*) = \frac{\sqrt{\kappa_h \kappa_{h,s}}}{\sqrt{\kappa_h} + 1} \quad \textit{and} \quad c_s(\tilde{\alpha}^*) = \frac{\sqrt{\kappa_h} - 1}{\sqrt{\kappa_h \kappa_{h,s}}}.$$

Proof. The equalities follow from straightforward computations. □

Obviously, at each step of the HSS iteration for the linear system (3.1) we only need to solve the linear sub-system with its coefficient matrix being the symmetric positive definite one $\tilde{\alpha}I + D + T$. In fact, the linear sub-system can be solved exactly by the Cholesky factorization method which is effective for the small dense symmetric positive definite linear system. For the large linear system, however, this will not be the case. A remedy may be using some Krylov subspace methods such as the CG method to solve the first linear sub-system as its inner iteration processes at each step of the outer HSS iteration. This result in the following PIHSS iteration for solving the system of linear equations (3.1).

The PIHSS iteration method for the linear system (3.1). Given an initial guess $\bar{u}^{(0)}$, for $k = 0, 1, \ldots$, until $\{\bar{u}^{(k)}\}$ converges, compute $\bar{u}^{(k+\frac{1}{2})}$ approximately from

$$(\tilde{\alpha}I + D + T)\bar{u}^{(k+\frac{1}{2})} \approx (\tilde{\alpha} - i\eta)\bar{u}^{(k)} + b$$

by employing the CG method with $\bar{u}^{(k)}$ as the initial guess; then solve $\bar{u}^{(k+1)}$ exactly from

$$\bar{u}^{(k+1)} = \frac{1}{\tilde{\alpha} + i\eta}\big[(\tilde{\alpha}I - D - T)\bar{u}^{(k+\frac{1}{2})} + b\big],$$

where $\tilde{\alpha}$ is a given positive constant and I is the identity matrix.

The following lemma [6] describes convergence property of the CG method for the linear sub-system with its coefficient matrix being the symmetric positive definite one $\tilde{\alpha}I + D + T$, which is essential to establish convergence theorems for the PIHSS iteration method for the linear system (3.1).

Lemma 3.1. *Let $\bar{u}^{(k+\frac{1}{2})}$ be the μ_kth approximate solution generated by μ_kth step of CG iteration with an initial guess $\bar{u}^{(k)}$ for solving the symmetric positive definite sub-system of linear equations $(\tilde{\alpha}I+D+T)\bar{u} = (\tilde{\alpha} - i\eta)\bar{u}^{(k)} + b$ of the $(k+1)$th step of the HSS iteration for the linear system (3.1). Then it holds that*

$$\|\bar{u}^{(k+\frac{1}{2})} - \bar{u}^{(k+\frac{1}{2},*)}\|_2 \le \sigma_h(\tilde{\alpha}, \mu_k)\|\bar{u}^{(k)} - \bar{u}^{(k+\frac{1}{2},*)}\|_2,$$

where

$$\bar{u}^{(k+\frac{1}{2},*)} = (\tilde{\alpha}I + D + T)^{-1}\big[(\tilde{\alpha} - i\eta)\bar{u}^{(k)} + b\big]$$

and

$$\sigma_h(\tilde{\alpha}, \mu_k) = 2\Big(\frac{\sqrt{\frac{\tilde{\alpha}+\lambda_M}{\tilde{\alpha}+\lambda_1}} - 1}{\sqrt{\frac{\tilde{\alpha}+\lambda_M}{\tilde{\alpha}+\lambda_1}} + 1}\Big)^{\mu_k}.$$

In particular, when $\tilde{\alpha} = \tilde{\alpha}^* = \sqrt{\lambda_1\lambda_M}$,

$$\sigma_h(\tilde{\alpha}^*, \mu_k) = 2\Big(\frac{\sqrt[4]{\kappa_h} - 1}{\sqrt[4]{\kappa_h} + 1}\Big)^{\mu_k}.$$

Based on Theorem 3.1 and Lemma 3.1, we can demonstrate the convergence theorems for the PIHSS iteration method for the linear system (3.1).

Theorem 3.2. *Let $A \in \mathbb{C}^{M\times M}$ be defined in (3.2), $D + T$ and $i\eta I$ be its Hermitian and skew-Hermitian parts,respectively, and $\tilde{\alpha}$ be a positive constant. Let $\{\mu_k\}$ be a sequence of positive integers. If the iterative*

sequence $\{\bar{u}^{(k)}\}$ is generated by the PIHSS iteration for the linear system (3.1) from an initial guess $\bar{u}^{(0)}$, then it holds that

$$\|\bar{u}^{(k+1)} - u^*\|_2 \leq \Big[c_s(\tilde{\alpha})(1 + c_h(\tilde{\alpha}))\sigma_h(\tilde{\alpha}, \mu_k) + \rho(\tilde{\alpha})\Big]\|\bar{u}^{(k)} - u^*\|_2,$$

where u^* is the exact solution of the system of linear equations (3.1). Therefore, if there exists a non-negative constant $\sigma^{pihss}(\tilde{\alpha}) \in [0, 1)$ such that

$$c_s(\tilde{\alpha})(1 + c_h(\tilde{\alpha}))\sigma_h(\tilde{\alpha}, \mu_k) + \rho(\tilde{\alpha}) \leq \sigma^{pihss}(\tilde{\alpha}), \quad k = 0, 1, 2, \ldots,$$

then the iterative sequence $\{\bar{u}^{(k)}\}$ converges to u^* with a convergence factor being at most $\sigma^{pihss}(\tilde{\alpha})$.

Proof. For a fixed iterate index k, from the PIHSS iteration method for the linear system (3.1) and Lemma 3.1 we have

$$\begin{cases} \bar{u}^{(k+\frac{1}{2},*)} = (\tilde{\alpha}I + D + T)^{-1}[(\tilde{\alpha} - i\eta)\bar{u}^{(k)} + b], \\ \bar{u}^{(k+1)} = \frac{1}{\tilde{\alpha}+i\eta}[(\tilde{\alpha}I - D - T)\bar{u}^{(k+\frac{1}{2})} + b], \end{cases} \tag{3.3}$$

and

$$\|\bar{u}^{(k+\frac{1}{2})} - \bar{u}^{(k+\frac{1}{2},*)}\|_2 \leq \sigma_h(\tilde{\alpha}, \mu_k)\|\bar{u}^{(k)} - \bar{u}^{(k+\frac{1}{2},*)}\|_2. \tag{3.4}$$

Let u^* be the exact solution of the system of linear equations (3.1), then from (3.3), we have

$$\begin{aligned} \bar{u}^{(k)} - \bar{u}^{(k+\frac{1}{2},*)} &= \bar{u}^{(k)} - (\tilde{\alpha}I + D + T)^{-1}[(\tilde{\alpha} - i\eta)\bar{u}^{(k)} + b] \\ &= (\tilde{\alpha}I + D + T)^{-1}[(\tilde{\alpha}I + D + T)\bar{u}^{(k)} - (\tilde{\alpha} - i\eta)\bar{u}^{(k)} - b] \\ &= (\tilde{\alpha}I + D + T)^{-1}[(\tilde{\alpha}I + D + T) - (\tilde{\alpha}I - i\eta I)](\bar{u}^{(k)} - u^*) \\ &= [I - (\tilde{\alpha} - i\eta)(\tilde{\alpha}I + D + T)^{-1}](\bar{u}^{(k)} - u^*). \end{aligned} \tag{3.5}$$

The exact solution u^* satisfies the sub-systems of linear equations

$$\begin{cases} (\tilde{\alpha}I + D + T)u^* = (\tilde{\alpha} - i\eta)u^* + b, \\ u^* = \frac{1}{\tilde{\alpha}+i\eta}[(\tilde{\alpha}I - D - T)u^* + b]. \end{cases} \tag{3.6}$$

After subtracting (3.6) from (3.3), we obtain

$$\begin{cases} (\tilde{\alpha}I + D + T)(\bar{u}^{(k+\frac{1}{2},*)} - u^*) = (\tilde{\alpha} - i\eta)(\bar{u}^{(k)} - u^*), \\ (\bar{u}^{(k+1)} - u^*) = \frac{1}{\tilde{\alpha}+i\eta}(\tilde{\alpha}I - D - T)(\bar{u}^{(k+\frac{1}{2})} - u^*). \end{cases} \tag{3.7}$$

The equalities in (3.7) straightforwardly yield

$$\begin{aligned} \bar{u}^{(k+1)} - u^* &= \frac{1}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\bar{u}^{(k+\frac{1}{2})} - u^*) \\ &= \frac{1}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\bar{u}^{(k+\frac{1}{2})} - \bar{u}^{(k+\frac{1}{2},*)}) + \frac{1}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\bar{u}^{(k+\frac{1}{2},*)} - u^*) \\ &= \frac{1}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\bar{u}^{(k+\frac{1}{2})} - \bar{u}^{(k+\frac{1}{2},*)}) + \frac{\tilde{\alpha} - i\eta}{\tilde{\alpha} + i\eta}(\tilde{\alpha}I - D - T)(\tilde{\alpha}I + D + T)^{-1}(\bar{u}^{(k)} - u^*). \end{aligned} \tag{3.8}$$

From (3.8), (3.4) and (3.5) it then follows that

$$\begin{aligned}\|\bar{u}^{(k+1)}-u^*\|_2 &\leq \|\frac{1}{\tilde{\alpha}+i\eta}(\tilde{\alpha}I-D-T)\|_2\|\bar{u}^{(k+\frac{1}{2})}-\bar{u}^{(k+\frac{1}{2},*)}\|_2\\ &\quad+\|\frac{\tilde{\alpha}-i\eta}{\tilde{\alpha}+i\eta}(\tilde{\alpha}I-D-T)(\tilde{\alpha}I+D+T)^{-1}\|_2\|\bar{u}^{(k)}-u^*\|_2\\ &\leq c_s(\tilde{\alpha})\sigma_h(\tilde{\alpha},\mu_k)\|\bar{u}^{(k)}-\bar{u}^{(k+\frac{1}{2},*)}\|_2+\rho(\tilde{\alpha})\|\bar{u}^{(k)}-u^*\|_2\\ &\leq c_s(\tilde{\alpha})\sigma_h(\tilde{\alpha},\mu_k)(1+c_h(\tilde{\alpha}))\|\bar{u}^{(k)}-u^*\|_2+\rho(\tilde{\alpha})\|\bar{u}^{(k)}-u^*\|_2\\ &\leq \left[c_s(\tilde{\alpha})\sigma_h(\tilde{\alpha},\mu_k)(1+c_h(\tilde{\alpha}))+\rho(\tilde{\alpha})\right]\|\bar{u}^{(k)}-u^*\|_2.\end{aligned}$$

□

Theorem 3.2 presents an estimate for the contraction factor of the PIHSS iteration for the linear system (3.1). Moreover, we can take $\tilde{\alpha}=\tilde{\alpha}^*$ which is the optimal parameter to further minimize the contraction factor and consequently, accelerate the convergence speed of the PIHSS iteration for solving the linear system (3.1). More precisely, we have the following theorem.

Theorem 3.3. *Let $A\in\mathbb{C}^{M\times M}$ be defined in (3.2), $D+T$ and $i\eta I$ be its Hermitian and skew-Hermitian parts, respectively, and $\tilde{\alpha}=\tilde{\alpha}^*=\sqrt{\lambda_1\lambda_M}$. Let $\{\mu_k\}$ be a sequence of positive integers. If the iterative sequence $\{\bar{u}^{(k)}\}$ is generated by the PIHSS for the linear system (3.1) from an initial guess $\bar{u}^{(0)}$, then it holds that*

$$\|\bar{u}^{(k+1)}-u^*\|_2\leq\left[2\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h\kappa_{h,s}}}(1+\frac{\sqrt{\kappa_h\kappa_{h,s}}}{\sqrt{\kappa_h}+1})(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})^{\mu_k}+\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}\right]\|\bar{u}^{(k)}-u^*\|_2.$$

Therefore, if μ_k is chosen such that

$$2\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h\kappa_{h,s}}}(1+\frac{\sqrt{\kappa_h\kappa_{h,s}}}{\sqrt{\kappa_h}+1})(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})^{\mu_k}<\frac{2}{\sqrt{\kappa_h}+1},k=0,1,2,\ldots,$$

then the iterative sequence $\{\bar{u}^{(k)}\}$ converges to the exact solution u^* of the system of linear equations (3.1).

We only substitute $c_s(\tilde{\alpha}),c_h(\tilde{\alpha}),\rho(\tilde{\alpha}),\sigma_h(\tilde{\alpha},\mu_k)$ by $c_s(\tilde{\alpha}^*),c_h(\tilde{\alpha}^*),\rho(\tilde{\alpha}^*),\sigma_h(\tilde{\alpha}^*,\mu_k)$ and then easily obtain Theorem 3.3.

The contraction factor of the PIHSS iteration method for the linear system (3.1) is bounded by

$$2\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h\kappa_{h,s}}}(1+\frac{\sqrt{\kappa_h\kappa_{h,s}}}{\sqrt{\kappa_h}+1})(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})^{\mu_k}+\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}\tag{3.9}$$

whose dominant term $\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}$ is approximately equal to the contraction factor of CG applied to symmetric definite system of linear equations $(D+T)y=b$. Evidently, the best possible bound of the contraction factor of the PIHSS iteration method for the linear system (3.1) is $\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}$. To make the bound of the contraction factor (3.9) approach to $\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}$ quickly and economically with increasing of μ_k, we should choose the inner CG iteration step μ_k at the kth outer iterate such that the factor $(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})^{\mu_k}$ approach to zero quickly. Then μ_k needs to be larger in theory, but this will lead to large computation increase actually. Thus, these two factors should be well balanced.

If μ_k is chosen so that

$$2\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h\kappa_{h,s}}}(1+\frac{\sqrt{\kappa_h\kappa_{h,s}}}{\sqrt{\kappa_h}+1})(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})^{\inf\{\mu_k\}_{k\geq 0}}+\frac{\sqrt{\kappa_h}-1}{\sqrt{\kappa_h}+1}<1,$$

or in other words

$$\mu_k \geq \frac{\ln\left(\frac{\sqrt{\kappa_h\kappa_{h,s}}}{(\sqrt{\kappa_h}-1)(\sqrt{\kappa_h}+1+\sqrt{\kappa_h\kappa_{h,s}})}\right)}{\ln(\frac{\sqrt[4]{\kappa_h}-1}{\sqrt[4]{\kappa_h}+1})},$$

then the PIHSS iteration method converges to the exact solution u^* of the system of linear equations (3.1).

4 Numerical results

In this section, we carry out numerical experiments to study the performances of the HSS and the PIHSS iteration methods. We employ the BiCGSTAB method, the SSOR iteration method, the HSS iteration method and the PIHSS iteration method to solve the linear system (3.1). The parameters involved in the SSOR, the HSS and the PIHSS iteration methods are set to be the experimentally optimal ones. All numerical experiments are started from the zero vector, performed in MATLAB with machine precision 10^{-16}. The outer PIHSS iteration for the linear system (3.1) are terminated when the current iterate satisfies

$$\frac{\|r^{(k)}\|_2}{\|r^{(0)}\|_2}<10^{-6},$$

where $r^{(k)}$ is the residual vector of the kth outer PIHSS iterate and $r^{(0)}$ is the initial residual vector. That is, $r^{(k)}=b-A\bar{u}^{(k)}$ and $r^{(0)}=b-A\bar{u}^{(0)}$, where $\bar{u}^{(0)}$ and $\bar{u}^{(k)}$ are the initial guess and the approximate solution of the kth outer PIHSS iterate, respectively.

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

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

subjected to the initial boundary value conditions

$$u(x,0)=\mathrm{sech}(x)\cdot\exp(2ix),\quad u(-20,t)=u(20,t)=0.$$

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

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

we take the initial boundary value conditions in the form

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

In our implementations, the inner CG iteration for the first linear sub-system in the PIHSS method are terminated if the current residuals of the inner iterate satisfy

$$\frac{\|p^{(k-1,j)}\|_2}{\|r^{(k-1)}\|_2}<10^{-\delta},$$

Table 1: Numerical results for Example 1 when $\alpha = 1.2$

M	BiCGSTAB		SSOR		HSS		PIHSS			
							$\delta = 2$		$\delta = 3$	
	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU
800	46	0.27	21	0.54	47	0.40	54	0.24	48	0.28
1600	70	1.76	36	3.67	39	1.50	42	0.69	39	0.76
3200	141	14.37	55	30.28	28	4.54	38	2.72	29	3.22
5000	186	46.86	71	93.46	23	11.36	27	8.16	24	10.71

Table 2: Numerical results for Example 1 when $\alpha = 1.7$

M	BiCGSTAB		SSOR		HSS		PIHSS			
							$\delta = 2$		$\delta = 3$	
	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU
800	49	0.30	30	0.77	54	0.46	59	0.30	56	0.36
1600	101	2.53	55	5.65	45	1.68	48	0.86	43	0.91
3200	187	19.09	96	50.84	32	5.09	40	3.89	34	4.35
5000	236	34.64	108	148.37	26	12.16	34	10.20	25	11.09

where $p^{(k-1,j)}$ is the residual of the jth inner CG iterate in the kth outer PIHSS iterate. In other words, $p^{(k-1,j)} = (\tilde{\alpha} - i\eta)\bar{u}^{(k-1)} + b - (\tilde{\alpha}I + D + T)\bar{u}^{(k+\frac{1}{2},j)}$, where $\bar{u}^{(k+\frac{1}{2},j)}$ is the jth iteration approximate solution of the first linear sub-system in the PIHSS iteration by the CG method. Here δ is the control tolerances for the CG iteration about the first linear sub-problem in the PIHSS method. δ should be chosen as large as possible in theory. However, the good convergence properties of the PIHSS iteration method are preserved even when the inner solves are performed to rather low accuracy, we take δ to be 2 and 3 in our tests.

The numerical results are listed in Tables 1−4, where "M" denotes the number of spatial grid points, "Iter" denotes the iteration steps of the BiCGSTAB method, the SSOR iteration method and the HSS iteration method, and the outer iteration step of the PIHSS iterate, and "CPU" denotes the total CPU time in seconds for solving the discretized system, and "α" denotes the order of the space fractional CNLS equations.

In Tables 1−2 and Tables 3−4 we list the iteration steps and the CPU time in seconds for the BiCGSTAB method, the SSOR iteration method, the HSS iteration method and the PIHSS iteration method for Examples 1 and 2 when $\alpha = 1.2$ and $\alpha = 1.7$ with respect to different spatial grids. The time step sizes for Examples 1 and 2 are all set to be 0.05. Because the numerical results for different values of α are similar, we only gave the numerical results for $\alpha = 1.2$ and $\alpha = 1.7$. The GMRES method are not convergent when solving the Examples 1 and 2, so its numerical results are not listed in the tables.

From these tables we can see that the iteration steps of the BiCGSTAB and SSOR methods are increasing quickly as the spatial grid points increases, but those of the HSS and PIHSS iteration methods are decreasing. The HSS and the PIHSS iteration methods which exhibit excellent performance outperform the BiCGSTAB and SSOR methods in terms of both iteration step and CPU time. The numerical results for the BiCGSTAB and SSOR methods are unsatisfactory which may be caused by the bad condition number of the coefficient matrix of the discretized linear system. To achieve the prescribed convergence criterion, the HSS iteration method requires less iteration step but more computing time than the PIHSS

Table 3: Numerical results for Example 2 when $\alpha = 1.2$

M	BiCGSTAB		SSOR		HSS		PIHSS			
							$\delta = 2$		$\delta = 3$	
	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU
800	44	0.26	21	0.56	43	0.37	48	0.18	45	0.18
1600	72	1.82	36	3.73	36	1.35	45	0.79	39	0.82
3200	96	10.07	55	32.71	27	5.22	42	3.75	35	4.43
5000	226	58.17	71	78.76	22	11.27	39	7.39	32	9.12

Table 4: Numerical results for Example 2 when $\alpha = 1.7$

M	BiCGSTAB		SSOR		HSS		PIHSS			
							$\delta = 2$		$\delta = 3$	
	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU	Iter	CPU
800	73	0.45	30	0.78	49	0.42	56	0.29	51	0.38
1600	80	2.01	55	5.91	42	1.56	52	1.05	45	1.11
3200	115	12.22	96	54.36	31	5.95	46	4.79	37	5.39
5000	243	62.35	108	151.40	25	12.03	38	8.45	29	10.25

iteration method, and the PIHSS iteration method with $\delta = 3$ requires less iteration step but more computing time than the PIHSS iteration method with $\delta = 2$. Therefore, among all the iterations, the HSS iteration method is the most effective in terms of the iteration step, and the PIHSS iteration method with $\delta = 2$ is the most effective in terms of the CPU time.

5 Concluding remarks

In this paper, the HSS iteration method and the PIHSS iteration method are employed to solve the complex symmetric linear systems arising from the discretization of the space fractional CNLS equations. The coefficient matrix of the linear system is equal to the sum of the complex scaled identity matrix and the symmetric positive definite diagonal-plus-Toeplitz matrix. In the inner iteration processes of the PIHSS iteration method, the shifted Hermitian sub-systems are solved by the CG method. Both theoretical analyses and numerical experiments demonstrate that the HSS iteration and the PIHSS iteration for solving the linear system (3.1) are feasible and efficient. Moreover, we can also employ the preconditioned CG methods [13–15, 17] to solve the shifted Hermitian sub-system at each step of the PIHSS iteration, and give the same convergence theory. We remark that, instead of HSS method and PIHSS method, the preconditioned HSS iterations to speed up the convergence rate of the HSS method have been studied in [7, 8].

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