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Error Estimates of Operator Splitting Spectral Method for Semiclassical Sub-Diffusive Gross-Pitaevskii Equation

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Abstract. Nonlinear Gross-Pitaevskii-type models are frequently seen in the fields of Bose-Einstein condensation and quantum mechanics. We derive error estimates for the Lie-Trotter operator splitting spectral method for semiclassical sub-diffusive Gross-Pitaevskii equation in the unbounded domain or with the periodic boundary condition. After establishing a priori estimates for the analytic solution in fractional Sobolev space, the local error estimates for the Lie-Trotter splitting operator method are derived. The related estimates for the Lie commutator of nonlocal linear operator and nonlinear operator play key roles in deriving the local error estimates. We then obtain the global error bounds for the fully discrete scheme based on the space approximation with mapped Chebyshev spectral-Galerkin methods in the case of the unbounded domain and with Fourier spectral methods in the case of the periodic boundary condition. Especially, their convergence orders with respect to the small (scaled) Planck constant ε are obtained for the first time under the framework of Wentzel-Kramers-Brillouin analysis. Numerical experiments verify and complement our theoretical results.

AMS subject classifications: 35Q55, 65M15, 65M12, 65J15, 65M70, 70K75

Key words: Lie-Trotter operator splitting, sub-diffusive Gross-Pitaevskii equation, semiclassical regime, error estimates, mapped Chebyshev spectral-Galerkin methods, Fourier spectral methods.

1 Introduction

The aim of this article is to derive error estimates for Lie-Trotter operator splitting Fourier-like spectral methods for the semiclassical sub-diffusive Gross-Pitaevskii equation

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$$i\varepsilon\partial_t u^\varepsilon = \frac{\varepsilon^{2s}}{2}(-\Delta)^s u^\varepsilon + Vu^\varepsilon + \lambda|u^\varepsilon|^2 u^\varepsilon, \quad (x,t)\in\mathbb{R}^d\times(0,T], \tag{1.1}$$

$$u^\varepsilon(x,0) = u_0^\varepsilon(x), \qquad x\in\mathbb{R}^d \tag{1.2}$$

in the unbounded domains $\mathbb{R}^d$ or with the periodic boundary condition

$$u(x+L\mathbf{n}_j,t) = u(x,t), \quad j=1,2,3,\dots, \tag{1.3}$$

where ε is a small (scaled) Planck constant, $0<\varepsilon<1$, i is the imaginary unit, $u^\varepsilon = u^\varepsilon(x,t)$ is the quantum mechanical wave function for the space variable x and the time variable t, the real value function $V=V(x)$ is electrostatic potential, the parameter $s\in(0,1]$ describes the fractional dispersive nature of the equation, and $\mathbf{n}_j$ is an orthonormal basis of $\mathbb{R}^d$ for $d=1,2,3$ (the vector with all entries equal to 0 but the j-th equal to 1). In addition, $\lambda=\pm1$ distinguishes between focusing (repulsive) $\lambda=-1$ and defocusing (attractive) $\lambda=1$ nonlinearities. The classical Schrödinger equation plays central role in a wide range of applications and is originally derived from quantum mechanics. The space-fractional Schrödinger equation (i.e. $V\equiv 0$) with $1/2<s<1$ was first introduced in [32, 33] by generalizing the Feynman path integral over Lévy trajectories. Recently, it has also been used in the mathematical description of Boson-stars [17, 35] and in the continuum limit of discrete models with long range interaction [29]. The time-dependent Gross-Pitaevskii equation (SDGPE) also arises in the description of the macroscopic wave function of a Bose-Einstein condensate when $s=1$. There has been much research on the existence of standing waves of such equation and its fractional dynamics (see, e.g. [18, 19, 30, 45]). Since it is difficult to find the solutions to such type of equations, several numerical methods have been proposed to solve numerically them; see, e.g. finite difference methods [16, 28, 41, 49–51, 58], time-splitting spectral methods [4, 5, 14, 31, 37, 48, 56], Galerkin finite element method [36], and Fourier pseudo-spectral method [22], and so on.

These numerical methods analyzed in the literature are based on the assumption that the Planck constant ε is large. However, the Planck constant ε is small in the practical quantum mechanics. In this case, i.e. in the semiclassical regime, designing efficient numerical methods and producing an accurate approximation of the solutions for time-dependent Schrödinger equation is a formidable mathematical challenge (see, e.g. [6, 15, 25–27, 34, 38, 39, 53]). As one of effective numerical methods for solving standard semiclassical nonlinear Schrödinger equation (NLS, that is, $s=1$; see, e.g. [7, 8, 39]), operator splitting spectral methods have been examined by several authors for solving semiclassical NLS (see, e.g. [4, 14, 31]). For the standard Gross-Pitaevskii equation (GPE), the splitting methods are mainly used to deal with the nonlinear terms (see, e.g. [8, 38]). For the SDGPE (1.1), this kind of methods become more appealing for they allow us to effectively deal with the nonlocal operator and the nonlinear terms simultaneously. However, to the best of our knowledge, no work has been done on the error estimates of the operator splitting methods for the semiclassical SDGPE, and little is known about the convergence order of the operator splitting methods with respect to the time step-size Δt.

Let $t_n = n\Delta t$ with Δt being a time step-size. Wang *et al.* [53] derived the local error bound of Lie-Trotter operator splitting method for linear semiclassical fractional Schrödinger equation with $1/2 < s \leq 1$ in unbounded domains, which recovers the results obtained in [11, 12] for standard linear Schrödinger equation (i.e. $s = 1$)

$$\left\|u^n - u^\varepsilon(t_n)\right\|_{L^2(\mathbb{R}^d)} \leq C\frac{\Delta t^2}{\varepsilon}, \quad n \geq 1, \tag{1.4}$$

where $u^\varepsilon(t_n)$ denotes the value of the analytic solution $u^\varepsilon(x,t)$ at $t = t_n$, u^n denotes the splitting solution at $t = t_n$ satisfying exactly the Lie-Trotter splitting scheme (see Section 3) with exact previous step $u^\varepsilon(t_{n-1})$, and C is independent of ε and Δt. Based on this local error estimate, they also derived the global error bounds for the fully discrete Lie-Trotter splitting Fourier spectral method for semiclassical linear fractional Schrödinger equation with the periodic boundary condition on a truncated domain. As pointed out in [53], however, using the local error estimate obtained in the unbounded domain to derive the error estimate for the problem with the periodic boundary condition is not rigorous. In this paper, we will address this question and obtain the local error estimate of Lie-Trotter operator splitting method for semiclassical SDGPE in the unbounded domain or with the periodic boundary condition

$$\left\|u^n - u^\varepsilon(t_n)\right\|_{L^2(\mathbb{R}^d)} \leq C\frac{\Delta t^2}{\varepsilon^2}, \quad n \geq 1. \tag{1.5}$$

This will be done by generalizing the Lie commutator estimates of the nonlocal linear operator $(-\Delta)^s$ and the nonlinear operator $\lambda|u^\varepsilon|^2$ and can be viewed as an extension of those obtained in [12] for the standard nonlinear Schrödinger equation (i.e. $s = 1$). Due to the nonlocal property of the operator $(-\Delta)^s$, however, such an extension is not straightforward. It depends on a formula for the fractional Laplacian $(-\Delta)^s$ of the product of two functions and fractional mean value theorem.

Based on these local error estimates, the global error bounds for Lie-Trotter operator splitting mapped Chebyshev spectral-Galerkin methods (respectively Lie-Trotter operator splitting Fourier spectral methods) for semiclassical nonlinear SDGPE in the unbounded domain (respectively with the periodic boundary condition) are obtained

$$\left\|u^\varepsilon(t_n) - U^{\varepsilon,n}\right\|_{L^2} \leq C\left(\frac{\Delta t}{\varepsilon^2} + \frac{1}{(\varepsilon M)^{4s}}\right), \tag{1.6}$$

where $U^{\varepsilon,n}$ is the fully discrete approximation of $u^\varepsilon(t_n)$. Estimate (1.6) will be numerically illustrated by an example in Section 6.

The paper is organized as follows. We start in Section 2 by introducing some definitions and notations related to the semiclassical SDGPE and fractional Sobolev space and by presenting the a priori estimates for the analytic solution to the semiclassical SDGPE. By estimating Lie commutator of a nonlocal linear operator and a nonlinear operator under an abstract framework, in Section 3, we show that the local splitting error is bounded by $C\Delta t^2/\varepsilon^2$ for general nonlinear SDGPE and by $C\Delta t^2/\varepsilon$ for linear case, under the framework of Wentzel-Kramers-Brillouin (WKB) analysis. The global error bounds for the fully discrete mapped Chebyshev spectral-Galerkin methods are derived for SDGPE in the unbounded domain in Section 4. In this section, the global error estimates for the fully discrete Fourier spectral methods for semiclassical SDGPE with the periodic boundary condition are also discussed. It is essential to bear in mind that these theoretical results are obtained for the first time and not covered by those of published works. The numerical tests for the semiclassical SDGPE (1.1) both in the unbounded domain and with the periodic boundary condition are presented in Section 5 and verify our theoretical error bounds. In Section 6, we finally conclude with some remarks.

2 Semiclassical sub-diffusive Gross-Pitaevskii equation

In this section, we introduce the spectral fractional Laplace operator $(-\Delta)^s$ and derive the a priori estimates for the semiclassical SDGPE.

2.1 The spectral fractional Laplacian and the fractional Sobolev space

To treat both cases, the unbounded domain and the periodic domain, in uniform framework, we let $\Omega=\mathbb{R}^d$ or $\Omega=\mathbb{T}^d$ with $\mathbb{T}=\mathbb{R}/(2\pi\mathbb{Z})$ for the two different cases. Given $s\in(0,1]$, for u in the Schwartz class $\mathcal{S}(\mathbb{R}^d)$, the fractional Laplacian $(-\Delta)^s$ of u on unbounded domain is defined by the Fourier transform

$$(-\Delta)^s u := \mathcal{F}^{-1}\big(|\xi|^{2s}\widehat{u}(\xi)\big) = \frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\widehat{u}(\xi)|\xi|^{2s}e^{i\xi\cdot x}d\xi, \tag{2.1}$$

and on a periodic domain $\mathbb{T}^d$, is defined by the Fourier transform

$$(-\Delta)^s u := \mathcal{F}^{-1}\big(|\xi|^{2s}\widehat{u}(\xi)\big) = \frac{1}{(2\pi)^{d/2}}\sum_{\xi\in\mathbb{Z}^d}\widehat{u}(\xi)|\xi|^{2s}e^{i\xi\cdot x}, \tag{2.2}$$

where the Fourier transform $\widehat{u}\equiv\mathcal{F}u$ is given by

$$\widehat{u}(\xi) = \frac{1}{(2\pi)^{d/2}}\int_{\Omega}u(x)e^{-i\xi\cdot x}dx. \tag{2.3}$$

The fractional Laplacian $(-\Delta)^s$ of u can be also equivalently defined by the point-wise formula (see, e.g. [1,2,13,19,57])

$$(-\Delta)^s u(x) := C_{d,s}\, p.v.\int_{\mathbb{R}^d}\frac{u(x)-u(y)}{|x-y|^{d+2s}}dy, \tag{2.4}$$

and

$$(-\Delta)^s u(x) := C_{d,s}\sum_{\xi\in\mathbb{Z}^d} p.v.\int_{\mathbb{T}^d}\frac{u(x)-u(y)}{|x-y-\xi|^{d+2s}}dy, \tag{2.5}$$

respectively, where the notation $p.v.$ means that the integral is taken in the Cauchy principal value sense, namely

$$p.v.\int_{\mathbb{R}^d}\frac{u(x)-u(y)}{|x-y|^{d+2s}}dy=\lim_{\epsilon\to 0}\int_{\Omega\backslash B(x,\epsilon)}\frac{u(x)-u(y)}{|x-y|^{d+2s}}dy, \tag{2.6}$$

and $C_{d,s}$ is a normalization constant, given by

$$C_{d,s}:=\frac{4^s s\Gamma(s+d/2)}{\pi^{d/2}\Gamma(1-s)}.$$

Here $\Gamma(\cdot)$ is the usual Gamma function. Thus, for evaluating fractional diffusion of u at a spatial point, information involving all spatial points is needed. The reader may refer, e.g. to [13,43] for additional details.

We introduce the fractional Sobolev space (see, e.g. [13,23,52]) for $\Omega=\mathbb{R}^d$,

$$H^s(\Omega):=\left\{u\in L^2(\Omega):\int_\Omega(1+|\xi|^2)^s|\mathcal{F}u(\xi)|^2d\xi<+\infty\right\}, \tag{2.7}$$

which is endowed with the norm

$$\|u\|_{H^s(\Omega)}=\left(\int_\Omega(1+|\xi|^2)^s|\mathcal{F}u(\xi)|^2d\xi\right)^{\frac{1}{2}}.$$

For $\Omega=\mathbb{T}^d$, we have

$$H^s(\Omega):=\left\{u\in L^2(\Omega):\sum_{\xi\in\mathbb{Z}^d}\int_\Omega(1+|\xi|^2)^s|\mathcal{F}u(\xi)|^2d\xi<+\infty\right\}, \tag{2.8}$$

which is endowed with the norm

$$\|u\|_{H^s(\Omega)}=\left(\sum_{\xi\in\mathbb{Z}^d}\int_\Omega(1+|\xi|^2)^s|\mathcal{F}u(\xi)|^2d\xi\right)^{\frac{1}{2}}.$$

In this paper, we will frequently use the fractional Sobolev semi-norm

$$|u|_{H^s(\Omega)}=\left\|(-\Delta)^{\frac{s}{2}}u\right\|_{L^2(\Omega)},$$

and the inner product

$$(u,v)_{H^s(\Omega)}=\left((-\Delta)^{\frac{s}{2}}u,(-\Delta)^{\frac{s}{2}}v\right)_{L^2(\Omega)},\quad u,v\in H^s(\Omega).$$

For simplicity, in what follows $\|\cdot\|_{L^2(\Omega)}$ and the inner product $(\cdot,\cdot)_{L^2(\Omega)}$ will be denoted by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively.

2.2 Conservation properties of semiclassical SDGPE

Similar to the standard $(s=1)$ GPE, the SDGPE (1.1)-(1.2) has two important conserved quantities.

Lemma 2.1. *Let* $0<s\le 1$ *and* $u^\varepsilon(t)$ *solve the problem* (1.1)-(1.2). *Then*

$$\|u^\varepsilon(t)\| = \|u_0^\varepsilon\|, \quad \forall t\ge 0. \tag{2.9}$$

Proof. The proof is similar to that of the linear case given in [14]. Multiplying both sides of (1.1) by $\bar{u}^\varepsilon$, where $\bar{u}^\varepsilon$ is the complex conjugate of u^ε, integrating with respect to x, and taking the imaginary part yields

$$\frac{d}{dt}\|u(t)\|^2 = 0.$$

Then (2.9) is a direct result of the above equation. □

From (2.9), we know that the mass of the wave function of the SDGPE (1.1)-(1.2) is conserved for $t\ge 0$, similar to the standard $(s=1)$ GPE,

$$M^\varepsilon(t) = \|u^\varepsilon(t)\|^2 = \int_\Omega |u^\varepsilon(x,t)|^2 dx = \int_\Omega |u^\varepsilon(x,0)|^2 dx = M^\varepsilon(0). \tag{2.10}$$

The total energy (or Hamiltonian)

$$\mathcal{E}_s(t) = \int_\Omega \left(\frac{\varepsilon^{2s}}{2} \left|(-\Delta)^{\frac{s}{2}} u^\varepsilon\right|^2 + V|u^\varepsilon|^2 + \frac{\lambda}{2}|u^\varepsilon|^4 \right) dx \tag{2.11}$$

has been also proved to be conserved in [14].

Lemma 2.2 ([14])**.** *Let* $u^\varepsilon(t)$ *solve the problem* (1.1)-(1.2). *Then we have conservation of energy*

$$\mathcal{E}_s(t) = \mathcal{E}_s(0). \tag{2.12}$$

Proof. The proof of this lemma is quite similar to the proof given in [14] for linear case and so is omitted. □

On basis of two conservation properties, (2.9) and (2.12), we show the a priori estimates below, which is novel in semiclassical regime.

Theorem 2.1 ($H^s(\Omega)$ Estimate)**.** *Let* $0<s\le 1$. *Let* $u^\varepsilon(t)$ *solve the problem* (1.1)-(1.2) *and satisfy* $\|u^\varepsilon(t)\|_{L^4(\Omega)} \le \beta$ *for every* $t\in[0,T]$. *Suppose* $u_0^\varepsilon \in H^{2s}(\Omega)$ *satisfies* (2.18) *and* $V\in L^\infty(\Omega)\cap L^2(\Omega)$. *Then there exists a positive constant* δ_1, *independent of* $\varepsilon\in(0,1]$ *and* s *such that*

$$|u^\varepsilon(t)|_{H^s(\Omega)} \le \delta_1 \varepsilon^{-s} \tag{2.13}$$

for every $t\ge 0$ *and every* $\varepsilon>0$.

Proof. It follows from (2.9) and (2.12) that

$$\begin{aligned}\frac{\varepsilon^{2s}}{2}\left\|(-\Delta)^{\frac{s}{2}}u^\varepsilon\right\|^2 &\le \mathcal{E}_s(0)+C_0\|u^\varepsilon\|^2+|\lambda|\|u^\varepsilon\|^4_{L^4(\Omega)}\\ &=\mathcal{E}_s(0)+C_0\|u_0^\varepsilon\|^2+|\lambda|\|u^\varepsilon\|^4_{L^4(\Omega)},\end{aligned}\tag{2.14}$$

where $C_0=\|V\|_{L^\infty(\Omega)}$. Then we have

$$|u^\varepsilon(t)|^2_{H^s(\Omega)}\le C\Big(\left\|u_0^\varepsilon\right\|^2_{H^s(\Omega)}+\varepsilon^{-2s}\left\|u_0^\varepsilon\right\|^2+\varepsilon^{-2s}\left\|u_0^\varepsilon\right\|^4_{L^4(\Omega)}+\varepsilon^{-2s}\|u^\varepsilon\|^4_{L^4(\Omega)}\Big),\tag{2.15}$$

and therefore (2.13), for (2.18) and $\|u^\varepsilon(t)\|_{L^4(\Omega)}\le\beta$. □

Note that for the defocusing nonlinearities, we have $\|u^\varepsilon(t)\|_{L^4(\Omega)}\le\beta$ because of the energy conservation (2.12).

2.3 Wentzel-Kramers-Brillouin analysis

Given (1.1) with initial datum of WKB type

$$u^\varepsilon(x,0)=a_0(x)e^{\frac{i\phi_0(x)}{\varepsilon}},\tag{2.16}$$

the WKB method consists in seeking

$$u^\varepsilon(x,t)=a^\varepsilon(x,t)e^{\frac{i\phi(x,t)}{\varepsilon}},\quad a^\varepsilon\approx a+\varepsilon a^{(1)}+\varepsilon^2a^{(2)}+\cdots.\tag{2.17}$$

Then from (2.16) we assume that there are positive constant $\delta_s>0$ independent of ε and x such that

$$\left|u_0^\varepsilon\right|_{H^{ks}(\Omega)}\le\delta_s\varepsilon^{-ks},\quad s\in(1/2,1],\quad k=1,2.\tag{2.18}$$

With the WKB analysis carried out in [9], based on (2.17), we also assume that there are positive constants $\beta>0$ and $\gamma>0$ independent of ε,x,t such that

$$|u^\varepsilon|_{H^{ks}(\Omega)}\le\beta\varepsilon^{-ks},\quad s\in(1/2,1],\quad k=1,2,4,\quad\forall t\ge0,\tag{2.19}$$

and for $p=(p_1,p_2,\cdots,p_d),0\le p_j<1,j=1,\dots,d$,

$$\|\mathcal{D}^pu^\varepsilon(t)\|_{L^\infty(\Omega)}\le\gamma\varepsilon^{-\hat{p}},\quad\hat{p}=\max_{1\le j\le d}(p_j),\quad\forall t\ge0,\tag{2.20}$$

where $\mathcal{D}^p:=(\mathcal{D}^{p_1}_{x_1},\cdots,\mathcal{D}^{p_d}_{x_d})^\top$ with $\mathcal{D}^{p_j}_{x_j}$ being the partial Riemann-Liouville fractional derivative of order p_j and defined as [44],

$$\mathcal{D}^{p_j}_{x_j}f(x)=\frac{1}{\Gamma(1-p_j)}\frac{\partial}{\partial x_j}\int_0^{x_j}\frac{f(x_1,\cdots,x_{j-1},y,x_{j+1},\cdots,x_d)}{(x_j-y)^{p_j}}dy.\tag{2.21}$$

It should be pointed out that at present we can not obtain the estimate (2.19) and (2.20) for the nonlinear SDGPE (1.1)-(1.2) with $d=2,3$ based on WKB analysis. This will be a very involved work.

3 Local error estimates of operator splitting for semiclassical SDGPE

In this section, we consider the time discretization of semiclassical SDGPE (1.1) by exponential operator splitting methods and derive the local error estimates for Lie-Trotter operator splitting method. The method of operator splitting remains a very popular method both for analysis and numerical computations of partial differential equations (see, e.g. [21, 38, 54]). The basic idea of operator splitting is to split the original problem into two or several subproblems so that a separate treatment of the subproblems can be allowed for. In particular, this applies to the use of dedicated special numerical techniques for each of the subproblems. For the general review of splitting methods, we refer to [40].

3.1 Preparation: Lie derivatives

We use the calculus of Lie derivatives (see, e.g. [20, 24]). This calculus allows us to formally extend arguments for the less involved linear case to nonlinear problem, see also [38] and references given therein. The analytical solution of an initial value problem of the form

$$\frac{d}{dt}u(t)=F\big(u(t)\big), \quad t\geq 0, \quad u(0)=u_0, \tag{3.1}$$

involving an unbounded nonlinear operator $F:D(F)\subset\mathcal{X}\to\mathcal{X}$ defined on a nonempty subspace of the underlying Banach space $(\mathcal{X},\|\cdot\|_{\mathcal{X}})$ is formally given by

$$u(t)=\varphi_F^t(u_0), \quad t\geq 0, \tag{3.2}$$

the nonlinear evolution operator φ_F^t depends on time and acts on the initial value. For any unbounded nonlinear operator $G:D(G)\subset\mathcal{X}\to\mathcal{X}$, defined on a suitably chosen domain, we consider the Lie derivative D_F defined by

$$(D_FG)(v)=\frac{d}{dt}\Big|_{t=0}G\big(\varphi_F^t(v)\big)=G'(v)F(v), \quad v\in\mathcal{X} \tag{3.3}$$

with G' denoting the Fréchet derivative of G. Then the evolution operator and the Lie derivative associated with F are given through the relation $e^{tD_F}G(v)=G(\varphi_F^t(v))$ for $t\geq 0$. In particular, for the identity operator Id, the solution $\varphi_F^t(u_0)$ can be written as $e^{tD_F}\mathrm{Id}(u_0)$. The Lie commutator of two Lie derivatives is given by

$$[D_F,D_G](v)=D_FD_G(v)-D_GD_F(v)=G'(v)F(v)-F'(v)G(v), \tag{3.4}$$

more generally, the iterated Lie commutators are defined through

$$\mathrm{ad}_{D_F}^j(D_G)=\big[D_F,\mathrm{ad}_{D_F}^{j-1}(D_G)\big], \quad j\geq 1, \tag{3.5}$$

where $\mathrm{ad}_{D_F}^0(D_G)=D_G$.

3.2 Operator splitting for semiclassical SDGPE

To state the operator splitting methods for SDGPE (1.1)-(1.2), we explore an abstract formulation of ordinary differential equations on function spaces. The initial-boundary value problem (1.1)-(1.2) takes the form

$$\frac{d}{dt}u^\varepsilon(t)=Au^\varepsilon(t)+Bu^\varepsilon(t),\quad 0<t\le T,\quad u^\varepsilon(0)=u_0^\varepsilon \tag{3.6}$$

with the unbounded linear operator

$$A=-\frac{i\varepsilon^{2s-1}}{2}(-\Delta)^s \tag{3.7}$$

comprising the fractional Laplacian $(-\Delta)^s$ and unbounded nonlinear multiplication operator B with

$$Bu^\varepsilon=-\frac{iV}{\varepsilon}-i\lambda\varepsilon^{-1}|u^\varepsilon|^2u^\varepsilon, \tag{3.8}$$

involving the potential and the cubic nonlinearity. The analytic solution of the evolutionary problem (3.6) is (formally) given by

$$u^\varepsilon(t)=\mathrm{e}^{D_{A+B}t}u_0^\varepsilon:=\Phi_{A+B}(t)u_0^\varepsilon. \tag{3.9}$$

The operator splitting methods for solving semiclassical SDGPE (3.6) have the forms

$$u^\varepsilon(t_n)\approx\left(\mathrm{e}^{b_1D_B\Delta t}\mathrm{e}^{a_1D_A\Delta t}\cdots\mathrm{e}^{b_kD_B\Delta t}\mathrm{e}^{a_kD_A\Delta t}\right)^nu_0^\varepsilon,\quad t_n=n\Delta t,\quad \Delta t<1$$

with (real or complex) coefficients $(a_j,b_j)_{j=1}^k$. As the simplest operator splitting method, the Lie-Trotter splitting method has the form, with $k=1$ and $a_1=b_1=1$,

$$u^\varepsilon(t_n)\approx\left(\mathrm{e}^{D_B\Delta t}\mathrm{e}^{D_A\Delta t}\right)^nu_0^\varepsilon=\left(\Phi_B(\Delta t)\Phi_A(\Delta t)\right)^nu_0^\varepsilon,\quad t_n=n\Delta t,\quad \Delta t<1, \tag{3.10}$$

where $\Phi_A(t)$ and $\Phi_B(t)$ solve the following two subproblems, respectively,

$$\varepsilon\partial_tu^\varepsilon+\frac{i\varepsilon^{2s}}{2}(-\Delta)^su^\varepsilon=0,\qquad t\in(0,T], \tag{3.11}$$

$$\varepsilon\partial_tu^\varepsilon+iV(x)u^\varepsilon+i\lambda|u^\varepsilon|^2u^\varepsilon=0,\quad t\in(0,T]. \tag{3.12}$$

The solution operator $\Phi_A(t)$ of the free equation (3.11) can be expressed in terms of Fourier transforms as $\mathcal{F}^{-1}\mathrm{e}^{-i\varepsilon^{2s-1}|\xi|^{2s}t/2}\mathcal{F}$ and approximately computed by fast Fourier transform in a Fourier-like spectral method, whereas the exponential of B acts as pointwise multiplication operator. More precisely, since $|u^\varepsilon(x,t)|$ invariant in t, (3.12) can be integrated exactly, i.e.

$$u^\varepsilon(x,t)=\mathrm{e}^{(-i\varepsilon^{-1}V(x)-i\varepsilon^{-1}\lambda|u^\varepsilon(x,t_s)|^2)(t-t_s)}u^\varepsilon(x,t_s),\quad t\ge t_s\ge 0,\quad x\in\mathbb{R}^d. \tag{3.13}$$

These allow us to effectively deal with the nonlocal operator and the nonlinear terms simultaneously. We also assume that the solution of the free equation (3.11) satisfies the bound (2.20).

It is easy to show that the Lie-Trotter splitting conserves the mass, i.e.

$$M_n^\varepsilon = \left\| \left(\Phi_B(\Delta t)\Phi_A(\Delta t)\right)^n u_0^\varepsilon \right\|^2 = \|u^\varepsilon(x,0)\|^2 = M^\varepsilon(0), \quad n \geq 0. \tag{3.14}$$

Note also that the energy functions corresponding to (3.11) and (3.12) are preserved, respectively, i.e.

$$\begin{aligned}
\mathcal{E}_A(t) &= \int_\Omega \frac{\varepsilon^{2s}}{2} \left|(-\Delta)^{\frac{s}{2}} u^\varepsilon(t)\right|^2 dx = \frac{\varepsilon^{2s}}{2} \|u^\varepsilon(t)\|^2_{H^s(\Omega)} = \mathcal{E}_A(0), \\
\mathcal{E}_B(t) &= \int_\Omega \left(V|u^\varepsilon(t)|^2 + \frac{\lambda}{2}|u^\varepsilon(t)|^4 \right) dx = \mathcal{E}_B(0).
\end{aligned} \tag{3.15}$$

3.3 Lie commutator of nonlinear operators

To estimate the local error of Lie-Trotter operator splitting, we need to compute Lie commutator of linear operator A and nonlinear operator B. It follows from (3.7) and (3.8) that

$$A'(v) = -\frac{i\varepsilon^{2s-1}}{2}(-\Delta)^s, \quad B'(v) = -i\varepsilon^{-1}\left(V + 2\lambda|v|^2 + \lambda v^2\overline{(\cdot)}\right). \tag{3.16}$$

Then the Lie commutator can be calculated by

$$\begin{aligned}
[D_A, D_B](v) &= D_A D_B(v) - D_B D_A(v) = B'(v)A(v) - A'(v)B(v) \\
&= -\frac{\varepsilon^{2s-2}}{2}\big[V(-\Delta)^s v + 2\lambda|v|^2(-\Delta)^s v + \lambda v^2(-\Delta)^s \overline{v} \\
&\qquad - (-\Delta)^s(Vv + 2\lambda|v|^2 + \lambda v^2\overline{v})\big].
\end{aligned} \tag{3.17}$$

If B is linear, i.e. $\lambda = 0$, then for linear operators A and B, due to $A'(v) = A$ as well as $B'(v) = B$, the above relation reduces to

$$\begin{aligned}
[D_A, D_B](v) &= B'(v)A(v) - A'(v)B(v) = -[A,B]v = (BA - AB)v \\
&= \frac{\varepsilon^{2s-2}}{2}\left[v(-\Delta)^s V - I_s(V,v)\right],
\end{aligned} \tag{3.18}$$

where, for an unbounded domain,

$$I_s(u,v) = C_{d,s}\ p.v. \int_{\mathbb{R}^d} \frac{[u(x)-u(y)][v(x)-v(y)]}{|x-y|^{d+2s}} dy, \tag{3.19}$$

and for a periodic domain

$$I_s(u,v) = C_{d,s} \sum_{\xi \in \mathbb{Z}^d} p.v. \int_{\mathbb{T}^d} \frac{[u(x)-u(y)][v(x)-v(y)]}{|x-y-\xi|^{d+2s}} dy. \tag{3.20}$$

The relation (3.18) in an unbounded domain has been obtained in [53] for linear problems.

3.4 Local error estimates for Lie-Trotter operator splitting

In this section, we study the local error derived from operator splitting (3.10) for SDGPE (1.1)-(1.2). To do this, we need several lemmas and some assumptions. We first make several assumptions on the potential V and the wave function u^ε.

Following the spirit of [53], we assume that the potential $V(x)$ in (1.1) belongs to $L^\infty(\Omega)\cap H^{2s}(\Omega)$, and there exists a positive constant $C_1>0$ independent of ε such that the following Lipschitz condition holds:

$$|V(x)-V(y)|\leq C_1|x-y|. \tag{3.21}$$

We now present several useful lemmas.

Lemma 3.1 (see, e.g. [10,42]). *Let u and v be such that $(-\Delta)^s u$ and $(-\Delta)^s v$ exist in unbounded domain $\mathbb{R}^d$ and*

$$\int_{\mathbb{R}^d}\frac{\big|\big(u(x)-u(y)\big)\big(v(x)-v(y)\big)\big|}{|x-y|^{d+2s}}dy<\infty.$$

Then $(-\Delta)^s(uv)$ exists and is given by

$$(-\Delta)^s(uv)=u(-\Delta)^s v+v(-\Delta)^s u-I_s(u,v), \tag{3.22}$$

where $I_s(u,v)$ has been defined in (3.19).

When the fractional Laplacian $(-\Delta)^s$ is defined in a periodic domain, we can get the formula (3.22), too.

Lemma 3.2. *Let u and v be such that $(-\Delta)^s u$ and $(-\Delta)^s$ exist in a periodic domain $\mathbb{T}^d$ and*

$$\sum_{\xi\in\mathbb{Z}^d} p.v.\int_{\mathbb{T}^d}\frac{\big|\big(u(x)-u(y)\big)\big(v(x)-v(y)\big)\big|}{|x-y-\xi|^{d+2s}}dy<\infty.$$

Then $(-\Delta)^s(uv)$ exists and is given by (3.22) *with $I_s(u,v)$ being defined in* (3.20).

Proof. Using the definition (2.5) for the fractional Laplacian $(-\Delta)^s$ in periodic domain $\mathbb{T}^d$, the desired result (3.22) is obvious. □

The following fractional mean value theorem on multivariate function $f(x)$ has been shown in [53].

Lemma 3.3 (Fractional Mean Value Theorem, [53]). *Let $f:\Omega\to\Omega$ and its partial Riemann-Liouville fractional derivatives $\mathcal{D}_{x_k}^{\alpha_k}f(x):\Omega\to\Omega$, $k=1,2,\ldots,d$, be continuous in their all variables. Then we have, for $h=(h_1,h_2,\ldots,h_d)^\top$,*

$$f(x+h)=f(x)+\sum_{k=1}^{d}\frac{1}{\Gamma(1+\alpha_k)}h_k^{\alpha_k}\mathcal{D}_{x_k}^{\alpha_k}f(x+\theta_k^\top h),\quad 0<\alpha_k<1, \tag{3.23}$$

where $\theta_k=(\theta_{k1},\theta_{k2},\ldots,\theta_{kd})^\top$, $k=1,2,\ldots,d$ with $0\leq\theta_{kj}\leq 1$, $j=1,2,\ldots,d$.

Noting the regularity estimate presented in Theorem 2.1, now we have the following local error estimate for Lie-Trotter operator splitting method for semiclassical SDGPE.

Theorem 3.1 (Local Error Estimate)**.** *Let* $s\in(1/2,1)$. *Suppose* $V\in L^\infty(\Omega)\cap H^{2s}(\Omega)$ *satisfies* (3.21), $u_0^\varepsilon\in H^{2s}(\Omega)$ *satisfies* (2.18), *the solution to the nonlinear SDGPE* (1.1)-(1.2) *satisfies* (2.19) *and* (2.20), *and the solution of the free equation* (3.11) *satisfies* (2.20). *If* $\Delta t=\mathcal{O}(\varepsilon)$, *then the error after one step of the splitting* (3.10) *is bounded by*

$$\left\|\left(\Phi_{A+B}(\Delta t)-\Phi_B(\Delta t)\Phi_A(\Delta t)\right)u_0^\varepsilon\right\|\le C_2\frac{\Delta t^2}{\varepsilon}+C_3\frac{\Delta t^2}{\varepsilon^2}, \tag{3.24}$$

where C_2 *and* C_3 *are independent of* ε *and* Δt.

Proof. It follows from (3.9) and (3.10) that

$$\begin{aligned}&\left(\Phi_{A+B}(t)-\Phi_B(t)\Phi_A(t)\right)u_0^\varepsilon\\ =&\left[\mathrm{e}^{D_{A+B}t}-\mathrm{e}^{D_Bt}\mathrm{e}^{D_At}\right]u_0^\varepsilon\\ =&-\int_0^t\int_0^{\tau_1}\mathrm{e}^{\tau_1D_B}\mathrm{e}^{\tau_2D_A}[D_B,D_A]\mathrm{e}^{(\tau_1-\tau_2)D_A}\mathrm{e}^{(t-\tau_1)D_{A+B}}u_0^\varepsilon d\tau_2d\tau_1.\end{aligned} \tag{3.25}$$

From (3.17), employing Lemmas 3.1 and 3.2, we obtain

$$\begin{aligned}[D_B,D_A](v)=&\frac{\varepsilon^{2s-2}}{2}\big[V(-\Delta)^sv+2\lambda|v|^2(-\Delta)^sv+\lambda v^2(-\Delta)^s\overline{v}\\ &\qquad-(-\Delta)^s(Vv+2\lambda|v|^2+\lambda v^2\overline{v})\big]\\ =&\frac{\varepsilon^{2s-2}}{2}\big[-v(-\Delta)^sV+I_s(V,v)-2\lambda\overline{v}(-\Delta)^sv-2\lambda v(-\Delta)^s\overline{v}\\ &\qquad+2\lambda I_s(v,\overline{v})+\lambda\overline{v}I_s(v,v)+\lambda I_s(v^2,\overline{v})\big].\end{aligned} \tag{3.26}$$

With

$$v=\mathrm{e}^{(\tau_1-\tau_2)D_A}\mathrm{e}^{(t-\tau_1)D_{A+B}}u_0^\varepsilon=\mathrm{e}^{(\tau_1-\tau_2)D_A}u^\varepsilon(t-\tau_1),$$

in view of (2.20), we have $\|v\|_{L^\infty}\le\gamma$. Using the same argument as that in [53], we can bound $\|-v(-\Delta)^sV\|+\|I_s(V,v)\|$ as

$$\|-v(-\Delta)^sV\|+\|I_s(V,v)\|\le C\varepsilon^{1-2s}. \tag{3.27}$$

For the third and fourth terms on the right hand side of (3.26), we employ the a priori assumption (2.19) to obtain

$$\|\overline{v}(-\Delta)^sv\|+\|v(-\Delta)^s\overline{v}\|\le\|\overline{v}\|\|(-\Delta)^sv\|+\|v\|\|(-\Delta)^s\overline{v}\|\le C\varepsilon^{-2s}. \tag{3.28}$$

The remaining part of the proof is to estimate $|I_s(v,\bar{v})|,|I_s(v,v)|$, and $|I_s(v^2,\bar{v})|$. We only consider the case of unbounded domain $\Omega=\mathbb{R}^d$. The case of periodic domain $\Omega=\mathbb{T}^d$

is similar. We first estimate $|I_s(v,\bar{v})|$

$$|I_s(v,\bar{v})| \le \left| C_{d,s} p.v. \int_{\mathbb{R}^d} \frac{[v(x)-v(y)][\bar{v}(x)-\bar{v}(y)]}{|x-y|^{d+2s}} dy \right|. \tag{3.29}$$

Setting $y=x+\varepsilon q$, and employing fractional mean value Lemma 3.3, for $x \le \zeta \le x+\varepsilon q$, we have

$$\begin{aligned} |I_s(v,\bar{v})| &\le C_{d,s}\varepsilon^{-2s} \int_{\mathbb{R}^d} \frac{|v(x)-v(x+\varepsilon q)||\bar{v}(x)-\bar{v}(x+\varepsilon q)|}{|q|^{d+2s}} dq \\ &\le C_{d,s}\varepsilon^{-2s} \left(\int_{|q|\ge 1} \frac{\left|\mathcal{D}^{\beta_1} v(\zeta)(\varepsilon q)^{\hat{\beta}_1}\right| \left|\mathcal{D}^{\beta_1} \bar{v}(\zeta)(\varepsilon q)^{\hat{\beta}_1}\right|}{\Gamma(1+\hat{\beta}_1)|q|^{d+2s}} dq \right. \\ &\qquad \left. + \int_{|q|<1} \frac{\left|\mathcal{D}^{\beta_2} v(\zeta)(\varepsilon q)^{\hat{\beta}_2}\right| \left|\mathcal{D}^{\beta_2} \bar{v}(\zeta)(\varepsilon q)^{\hat{\beta}_2}\right|}{\Gamma(1+\hat{\beta}_2)|q|^{d+2s}} dq \right), \end{aligned} \tag{3.30}$$

where

$$\beta_1 = (\hat{\beta}_1, \ldots, \hat{\beta}_1)^\top, \quad \beta_2 = (\hat{\beta}_2, \ldots, \hat{\beta}_2)^\top.$$

Taking account into the assumptions, the bound (2.20), and $s \in (1/2,1)$, we can choose $0 < \hat{\beta}_1 < s$ and $s < \hat{\beta}_2 < 1$ such that

$$|I_s(v,\bar{v})| \le C_3 \varepsilon^{-2s} \tag{3.31}$$

with $C_3 > 0$, independent of ε. Similarly, we have $|I_s(v,v)| \le C_3\varepsilon^{-2s}$. For $|I_s(v^2,\bar{v})|$, since

$$\left| I_s(v^2,\bar{v}) \right| \le 2C_{d,s}\varepsilon^{-2s} \|v\|_{L^\infty(\mathbb{R}^d)} \int_{\mathbb{R}^d} \frac{|v(x)-v(x+\varepsilon q)||\bar{v}(x)-\bar{v}(x+\varepsilon q)|}{|q|^{d+2s}} dq, \tag{3.32}$$

we can obtain the same estimate as (3.31). Combining these estimates yields (3.24). This completes the proof. □

We end this section with some remarks.

The first remark is about linear problems. From the proof of Theorem 3.1, we can easily obtain the local error estimate for the Lie-Trotter splitting for linear Schrödinger equation

$$\left\| \left(\Phi_{A+B}(\Delta t) - \Phi_B(\Delta t)\Phi_A(\Delta t) \right) u_0^\varepsilon \right\| \le C_2 \frac{\Delta t^2}{\varepsilon}, \tag{3.33}$$

which has been obtained in [53].

The second remark is about the comparison of theoretical and numerical results. For semiclassical standard NLS (i.e. $s=1$) with initial data (2.16) whose first spatial derivative involving $1/\varepsilon$, Descombes and Thalhammer [12] showed that the local error can be expressed by

$$\left\| \left(\Phi_{A+B}(\Delta t) - \Phi_B(\Delta t)\Phi_A(\Delta t) \right) u_0^\varepsilon \right\| \le c_2 \frac{\Delta t^2}{\varepsilon^2} + c_3 \frac{\Delta t^3}{\varepsilon^3} + c_4 \frac{\Delta t^4}{\varepsilon^4} + c_5 \frac{\Delta t^5}{\varepsilon^5}, \tag{3.34}$$

and found that it is not consistent with some numerical results which display the error behaviour like $\mathcal{O}(\varepsilon^{-1})$ for a fixed time step-size $\Delta t = \mathcal{O}(\varepsilon)$. To explain the numerical observations, they gave a heuristic consideration. However, a numerical example presented in Section 5 illustrates that the local error estimate (3.24) is sharp for SDGPE with focusing nonlinearity, that is, the error behaviour of the Lie-Trotter operator splitting method with respect to the Planck constant ε is around $\mathcal{O}(\varepsilon^{-2})$ for a fixed time step-size $\Delta t = \mathcal{O}(\varepsilon)$. Note that when $\Delta t \leq \varepsilon$, the local error estimate (3.34) is identical with our error estimate (3.24) since in this case the term $c_2\Delta t^2/\varepsilon^2$ i s dominant in the error estimate (3.34). Thus, on the one hand, this verifies our theoretical results, but on the other hand this is may be an indicator that the presented local error estimate can be improved for some special cases.

4 Global error estimates for fully discrete approximation

In this section, we consider fully discrete approximation of SDGPE (1.1). With the operator splitting (3.10) for the time discretization, for the spatial discretization, it is natural to use the Fourier-like spectral method because of the definitions of fractional Laplacian (2.1) and (2.2).

4.1 Mapped Chebyshev spectral-Galerkin methods for SDGPE in unbounded domain

In this section, we apply the operator splitting together with the Fourier-like mapped Chebyshev spectral-Galerkin (MCSG) methods to SDGPE in an unbounded domain. For this purpose, we introduce mapped Chebyshev functions (MCFs) and some notations (see, e.g. [47, 48]).

4.1.1 The MCFs and MCF approximation

Let $T_n(y) = \cos(n\arccos(y)), y \in \omega := (-1,1)$, be the Chebyshev polynomial of degree n. Introducing the one-to-one algebraic mapping

$$x = \frac{y}{\sqrt{1-y^2}}, \quad y = \frac{x}{\sqrt{1+x^2}}, \quad x \in \mathbb{R}, \quad y \in \omega, \tag{4.1}$$

we define the MCFs as, for $x \in \mathbb{R}$ and integer $n \geq 0$,

$$\mathbf{T}_n(x) = \frac{\sqrt{1-y^2}}{\sqrt{c_n\pi/2}} T_n(y) = \frac{1}{\sqrt{c_n\pi/2}} \frac{1}{\sqrt{1+x^2}} T_n\left(\frac{x}{\sqrt{1+x^2}}\right).$$

Using this definition and the well-known properties of Chebyshev polynomials the following important properties of the MCFs can be shown (see [47, 48]).

Proposition 4.1. *The MCFs are orthonormal in $L^2(\mathbb{R})$, and we have*

$$S_{mn}=S_{nm}=\int_{\mathbb{R}}\mathbf{T}'_n(x)\mathbf{T}'_m dx$$
$$=\begin{cases}\dfrac{1}{c_n}\left(\dfrac{(4c_{n-1}-c_{n-2})(n-1)^2}{16}+\dfrac{(4c_{n+1}-c_{n+2})(n+1)^2}{16}-\dfrac{c_n}{4}\right), & \text{if} \quad m=n,\\ \dfrac{1}{\sqrt{c_nc_{n+2}}}\left(\dfrac{(c_n-c_{n+2})(n+1)}{8}-\dfrac{c_{n+1}(n+1)^2}{4}\right), & \text{if} \quad m=n+2,\\ \dfrac{1}{\sqrt{c_nc_{n+4}}}\left(\dfrac{c_{n+2}(n+1)(n+3)}{16}\right), & \text{if} \quad m=n+4.\end{cases} \tag{4.2}$$

Based on (4.2), we define $\mathbf{S}$ as a square matrix of order $M+1$ with entries given by (4.2), and let $\mathbf{I}$ the identity matrix of the same size. Let $\mathbf{E}=(e_{jk})_{j,k=1,\dots,N}$ be the matrix formed by the orthonormal eigenvectors of $\mathbf{S}$, and $\mathbf{\Sigma}=\mathrm{diag}\{\lambda_k\}$ be the diagonal matrix of the corresponding eigenvalues. Let us introduce the finite dimensional space

$$\mathbb{V}_M:=\{\mathbf{T}_m(x):0\le m\le M\},\quad M\ge 1.$$

Then $T_m(x)$ form a basis of $\mathbb{V}_M$, and we have the following property.

Proposition 4.2 (See [48]). *Let $\mathbf{E}=(\mathbf{e}_0,\mathbf{e}_1,\cdots,\mathbf{e}_M),\mathbf{e}_m=(e_{0m},e_{1m},\cdots,e_{Mm})^\top$, be the matrix of the eigenvectors of $\mathbf{S}$, i.e. $\mathbf{S}\mathbf{e}_m=\lambda_m\mathbf{e}_m$ for $0\le m\le M$. Define*

$$\widehat{\mathbf{T}}_m(x):=\sum_{k=0}^{M}e_{km}\mathbf{T}_k(x),\quad 0\le m\le M. \tag{4.3}$$

Then $\{\widehat{\mathbf{T}}_m\}_{m=0}^M$ form an equivalent basis of $\mathbb{V}_M$, and they are bi-orthogonal in the sense that

$$(\widehat{\mathbf{T}}_k,\widehat{\mathbf{T}}_m)=\delta_{km},\quad (\widehat{\mathbf{T}}'_k,\widehat{\mathbf{T}}'_m)=\lambda_k\delta_{km},\quad 0\le k,m\le M. \tag{4.4}$$

We further define the tensor product $\mathbb{V}_M^d$ of d copies of $\mathbb{V}_M$ as

$$\mathbb{V}_M^d:=\mathbb{V}_M\otimes\cdots\otimes\mathbb{V}_M$$

with $\mathbb{V}_M^1=\mathbb{V}_M$. Define the d-dimensional tensorial Fourier-like basis and denote the vector of the corresponding eigenvalues by

$$\widehat{\mathbf{T}}_m(x)=\prod_{j=1}^{d}\widehat{\mathbf{T}}_{m_j}(x_j),\quad x\in\mathbb{R}^d,\quad \lambda_m=(\lambda_{m_1},\cdots,\lambda_{m_d})^\top. \tag{4.5}$$

Define the index set Ψ_M as

$$\Psi_M:=\{m=(m_1,\cdots,m_d):0\le m_j\le M,1\le j\le d\}. \tag{4.6}$$

Then, accordingly, we have

$$\mathbb{V}_M^d = \{\widehat{\mathbf{T}}_m(x), m \in \Psi_M\}. \tag{4.7}$$

We consider d-dimensional L^2-orthogonal projection $\pi_M^d : L^2(\mathbb{R}^d) \to \mathbb{V}_M^d$ such that

$$\int_{\mathbb{R}^d} (\pi_M^d u - u)(x) v(x) dx = 0, \quad \forall v \in \mathbb{V}_M^d. \tag{4.8}$$

To estimate the projection error, we need introduce some notations and spaces of functions. Let

$$a(x_j) = \frac{dx_j}{dy_j} = (1+x_j)^{\frac{3}{2}}, \quad 1 \le j \le d.$$

We define the differential operators

$$\begin{aligned}
&\mathbf{D}_{x_j} u := \partial_{x_j}\{(1+x_j)^{\frac{1}{2}} u\} \frac{dx_j}{dy_j} = a(x_j) \partial_{x_j}\{(1+x_j)^{\frac{1}{2}} u\}, \\
&\mathbf{D}_{x_j}^{k_j} u := a(x_j) \partial_{x_j}\Big\{ a(x_j) \partial_{x_j}\Big\{ \cdots \{ a(x_j) \partial_{x_j}\{(1+x_j)^{\frac{1}{2}} u\}\} \cdots \Big\}\Big\}, \quad k_j \ge 1.
\end{aligned}$$

For the index $k = (k_1, k_2, \cdots, k_d)^\top$, we further introduce the differential operator

$$\mathbf{D}_x^k = \mathbf{D}_{x_1}^{k_1} \cdots \mathbf{D}_{x_d}^{k_d} u.$$

Then with the weight function $\rho^k(x) = \prod_{j=1}^d (1+x_j^2)^{-k_j}$, we define the d-dimensional Sobolev space

$$B^r(\mathbb{R}^d) = \{ u : \mathbf{D}_x^k u \in L^2_{\rho^{k+1}}(\mathbb{R}^d), 0 \le |k|_1 \le r \}, \quad r = 0,1,2,\ldots, \tag{4.9}$$

equipped with the norm and semi-norm

$$\|u\|_{B^r(\mathbb{R}^d)} = \left(\sum_{0 \le |k|_1 \le r} \big\| \mathbf{D}_x^k u \big\|^2_{L^2_{\rho^{1+k}}(\mathbb{R}^d)} \right)^{\frac{1}{2}}, \quad |u|_{B^r(\mathbb{R}^d)} = \left(\sum_{j=1}^d \big\| \mathbf{D}_{x_j}^k u \big\|^2_{L^2_{\rho^{1+r\mathbf{n}_j}}(\mathbb{R}^d)} \right)^{\frac{1}{2}}.$$

Then the projection error in the fraction Sobolev norm, i.e. $\|\pi_M^d u - u\|_{H^s(\mathbb{R}^d)}$, has been obtained in [48].

Lemma 4.1 ([48]). *If $u \in B^r(\mathbb{R}^d)$ with integer $m \ge 1$, then we have*

$$\big\| \pi_M^d u - u \big\|_{H^s(\mathbb{R}^d)} \le c M^{s-r} |u|_{B^r(\mathbb{R}^d)}, \quad 0 \le s \le 1, \tag{4.10}$$

where c is a positive constant independent of M and u.

To estimate the error of the interpolation operator, consider the Chebyshev-Gauss quadrature nodes $\{y_j\}_{j=0}^M$ and weights $\{\sigma_j\}_{j=0}^M$ on $\omega=(-1,1)$. The mapped nodes and weights will be denoted by

$$x_j=\frac{y_j}{\sqrt{1-y_j^2}},\quad \rho_j=\frac{\sigma_j}{1-y_j^2},\quad 0\le j\le M. \tag{4.11}$$

After introducing the one-dimensional interpolation operator $I_M: C(\mathbb{R})\to\mathbb{V}_M$ such that

$$I_M u(x_j)=u(x_j),\quad 0\le j\le M, \tag{4.12}$$

we consider the d-dimensional MCF interpolation $I_M^d: C(\mathbb{R}^d)\to\mathbb{V}_M^d$,

$$I_M^d u(x_j)=I_M^{(1)}\circ\cdots\circ I_M^{(d)}u(x_j),\quad j\in\Psi_M, \tag{4.13}$$

where $I_M^{(k)}, 1\le k\le d$, is the interpolation along x_k-direction, and introduce a second seminorm of $B^r(\mathbb{R}^d)$ for $r\ge 1$ as follows:

$$[[u]]_{B^r(\mathbb{R}^d)}:=\left\{|u|_{B^r(\mathbb{R}^d)}+\sum_{j=1}^d\sum_{m\neq j}\left\|\mathbf{D}_{x_m}^{r-1}\mathbf{D}_{x_j}u\right\|^2_{L^d_{\rho^{1+(r-1)\mathbf{n}_k+\mathbf{n}_j}}(\mathbb{R}^d)}\right\}. \tag{4.14}$$

Then the interpolation error can be bounded as follows.

Lemma 4.2 ([48]). *If $u\in B^r(\mathbb{R}^d)$ with integer $r\ge 2$, then we have*

$$\left\|I_M^d u-u\right\|_{L^2(\mathbb{R}^d)}\le cM^{-r}[[u]]_{B^r(\mathbb{R}^d)}, \tag{4.15}$$

where c is a positive constant independent of M and u.

4.1.2 Mapped Chebyshev spectral-Galerkin methods for SDGPE

Now we consider the fully discrete approximation of SDGPE based on Lie-Trotter operator splitting and mapped Chebyshev spectral-Galerkin methods. We seek $U_M^{\varepsilon,n}(x)\in\mathbb{V}_M^d$ as an approximate solution to subproblem (3.11) in unbounded domain such that

$$i\varepsilon\big(\partial_t u_M^\varepsilon,v\big)=\big(Au_M^\varepsilon,v\big)=\frac{\varepsilon^{2s}}{2}\big((-\Delta)^s u_M^\varepsilon,v\big),\quad \forall v\in\mathbb{V}_M^d. \tag{4.16}$$

Using the Fourier-like MCF basis, we write

$$u_M^\varepsilon(x,t)=\sum_{k\in\Psi_M}\hat{u}_k^\varepsilon(t)\widehat{\mathbf{T}}_k(x),\quad x\in\mathbb{R}^d,\quad t\in[0,T]. \tag{4.17}$$

Substituting it into (4.16) and taking the inner product with $\widehat{\mathbf{T}}_m(x)$, in view of (4.4), yields

$$i\frac{\partial\hat{u}_m^\varepsilon(t)}{\partial t}=\frac{\varepsilon^{2s}}{2}|\lambda_m|_1^s\hat{u}_m^\varepsilon(t),\quad m\in\Psi_M. \tag{4.18}$$

As a consequence, we deduce from (4.18) that the solution for (4.16), i.e. the numerical solution of (3.11), is given by

$$\begin{aligned} u_M^\varepsilon(x,t) &= \mathrm{e}^{-iA(t-t_{n-1})} u_M^\varepsilon(x,t_{n-1}) \\ &= \sum_{k\in\Psi_M} \mathrm{e}^{-\frac{i\varepsilon^{2s}}{2}|\lambda_k|_1^s(t-t_{n-1})} \hat{u}_k^\varepsilon(t_{n-1}) \widehat{\mathbf{T}}_k(x), \quad t\geq t_{n-1}. \end{aligned} \tag{4.19}$$

Let $\{x_m\}_{m\in\Psi_M}$ be tensorial grids. We define the solution map related to (4.19)

$$\Phi_A^h(\Delta t)v(x) = \sum_{k\in\Psi_M} \mathrm{e}^{-\frac{i\varepsilon^{2s}}{2}|\lambda_k|_1^s\Delta t} \hat{v}_k \widehat{\mathbf{T}}_k(x), \tag{4.20}$$

where $\{\hat{v}_k\}$ are the MCF expansion coefficients computed from the sampling of $v\in\mathbb{V}_M^d$ on the grids $\{x_m\}_{m\in\Psi_M}$.

Now we consider the fully discrete approximation of the SDGPE (1.1)-(1.2) by the Lie-Trotter operator splitting together with MCSG method as follows, from time $t=t_{n-1}$ to $t=t_n$ for any $m\in\Psi_M$,

$$U_m^{\varepsilon,*} = \Phi_A^h(\Delta t) U_m^{\varepsilon,n-1}, \quad U_m^{\varepsilon,n} = \mathrm{e}^{-i\varepsilon^{-1}\Delta t(V+\lambda|U_m^{\varepsilon,*}|^2)} U_m^{\varepsilon,*} = \Phi_B^h(\Delta t) U_m^{\varepsilon,*}. \tag{4.21}$$

Let $\{x_k,\rho_k\}_{k\in\Psi_M}$ be the corresponding tensorial nodes and weights as in (4.11). We further define

$$\|U^{\varepsilon,n}\|_{l^2}^2 = \sum_{k\in\Psi_M} \left|U_k^{\varepsilon,n}\right|^2 \rho_k := \sum_{k_1=0}^{M_1} \cdots \sum_{k_d=0}^{M_d} U^n(x_{k_1},\cdots,x_{k_d})\rho_{k_1}\cdots\rho_{k_d}, \tag{4.22}$$

where $U_k^{\varepsilon,n} = U^{\varepsilon,n}(x_k)$. Then it is easy to show the stability of the fully discrete approximation scheme (4.21).

Lemma 4.3. *The Lie-Trotter operator splitting method has the normalisation conservation, i.e.*

$$\|U^{\varepsilon,n}\|_{l^2}^2 = \sum_{k\in\Psi_M} \left|U_k^{\varepsilon,n}\right|^2 \rho_k = \sum_{k\in\Psi_M} \left|u_0^\varepsilon(x_k)\right|^2 \rho_k = \left\|u_0^\varepsilon\right\|_{l^2}^2, \quad n\geq 0. \tag{4.23}$$

4.1.3 Global error estimates for Lie-Trotter operator splitting MCSG methods

To show the global error bound of the Lie-Trotter operator splitting MCSG methods, in view of (2.19), it is reasonable to assume that

$$|u^\varepsilon(x,t)|_{B^r(\mathbb{R}^d)} \leq C\varepsilon^{-r}, \quad [[u^\varepsilon(x,t)]]_{B^r(\mathbb{R}^d)} \leq C\varepsilon^{-r}. \tag{4.24}$$

With previous preparations, we have the following error estimates.

Theorem 4.1 (Global Error Estimates)**.** *Let $u^\varepsilon = u^\varepsilon(x,t)$ be the analytic solution of* (1.1)-(1.2) *in unbounded domain $\Omega = \mathbb{R}^d$, and $U^{\varepsilon,n}$ be the discrete approximation given by* (4.21)*. Assume that the potential function $V \in C^2(\Omega)\cap H^{2s}(\Omega)$, and the solution $u^\varepsilon \in H^{4s}(\Omega)$. If*

$$\Delta t = \mathcal{O}(\varepsilon), \quad h = \mathcal{O}(\varepsilon), \tag{4.25}$$

then we have

$$\left\| u^\varepsilon(t_n) - I_M^d U^{\varepsilon,n} \right\|_{l^2} \le C\left(\frac{\Delta t}{\varepsilon^2} + \frac{1}{(\varepsilon M)^{4s}} \right), \tag{4.26}$$

where C is independent of $\varepsilon, M, \Delta t$. Especially, if $\lambda \equiv 0$ (that is, the problem is linear), we have

$$\left\| u^\varepsilon(t_n) - I_M^d U^{\varepsilon,n} \right\|_{L^2(\Omega)} \le C\left(\frac{\Delta t}{\varepsilon} + \frac{1}{(\varepsilon M)^{4s}} \right), \tag{4.27}$$

where C is also independent of $\varepsilon, M, \Delta t$.

Proof. The proof of this theorem is almost the same as that of [53, Theorem 5.5]. The only difference is the local error estimate (3.24) for semiclassical SDGPE. □

4.2 Fourier spectral methods for SDGPE with periodic boundary condition

In this section, we consider applying the Lie-Trotter operator splitting Fourier spectral methods for SDGPE (1.1) with a periodic boundary condition.

We define the index set Ψ_M^* as

$$\Psi_M^* := \left\{ m = (m_1, \cdots, m_d) : -\frac{M}{2} \le m_j \le \frac{M}{2} - 1, 1 \le j \le d \right\}. \tag{4.28}$$

Let still $U_j^{\varepsilon,n}$ be an approximation of $u_j^{\varepsilon,n} = u^\varepsilon(x_j, t_n), x_j \in \Psi_M$. We combine the time-splitting (3.10) and spatial spectral discretization, resulting in the Lie-Trotter splitting Fourier spectral method for the SDGPE (1.1) with the periodic boundary condition as follows:

$$U_j^{\varepsilon,*} = \sum_{l \in \Psi_M^*} \mathrm{e}^{-i\varepsilon^{2s-1} l^{2s} \frac{\Delta t}{2}} \widehat{U}_l^{\varepsilon,n} \varphi_l(x_j), \quad j \in \Psi_M, \tag{4.29}$$

$$U_j^{\varepsilon,n+1} = \mathrm{e}^{-i(V(x_j) + \lambda |U_j^{\varepsilon,n}|^2)\frac{\Delta t}{\varepsilon}} U_j^{\varepsilon,*}, \quad j \in \Psi_M, \tag{4.30}$$

where $\varphi_l(x) = \mathrm{e}^{il(x+\pi)}$, $l \in \Psi_M^*$, and $\widehat{U}_l^{\varepsilon,n}$, the discrete Fourier coefficient of $U^{\varepsilon,n}$, are defined as

$$\widehat{U}_l^{\varepsilon,n} = \frac{1}{M^d} \sum_{j \in \Psi_M} U_j^{\varepsilon,n} \bar{\varphi}_l(x_j), \quad U_j^{\varepsilon,0} = u_0^\varepsilon(x_j), \quad l \in \Psi_M^*. \tag{4.31}$$

The method (4.29)-(4.30) is based on fact that $|U_j^{\varepsilon,n}|^2 = |U_j^{\varepsilon,n+1}|^2$ and therefore explicit. Since (4.30) integrates exactly (3.12), the only time discretization error of this method is the splitting error. We also note that the above algorithm can be rewritten in the abstract formula as

$$U_j^{\varepsilon,n+1} = \Phi_B^h(\Delta t)\Phi_A^h(\Delta t) U_j^{\varepsilon,n}, \quad j \in \Psi_M. \tag{4.32}$$

4.2.1 Interpolation operator and projection operator

Let us introduce the trigonometric interpolation operator $\mathcal{I}_M$ which is defined on Ψ_M by

$$\mathcal{I}_M u(x)=\sum_{l\in\Psi_M^*}\widehat{u}_l\varphi_l(x),\quad \widehat{u}_l=\frac{1}{M^d}\sum_{j\in\Psi_M}u(x_j)\bar{\varphi}_l(x_j),\quad l\in\Psi_M^*.$$

It is useful to note the following error estimate.

Lemma 4.4 (see, e.g. [46,55]). *Suppose that $u\in H^r(\Omega)$ with $r>0$, then the following estimate holds:*

$$\|\mathcal{I}_M u-u\|_{L^2(\Omega)}\leq C_4 M^{-r}\|u\|_{H^r(\Omega)}. \tag{4.33}$$

The following conservation property can be proved easily.

Theorem 4.2 (Mass Conservation, see [53]). *The operator splitting spectral scheme* (4.29)-(4.30) *conserves the discrete mass, i.e.*

$$\|U^{\varepsilon,n}\|_{l^2}=\left\|u_0^\varepsilon\right\|_{l^2},\quad n=1,2,\dots,N, \tag{4.34}$$

and consequently, in view of $\|\mathcal{I}_M u\|^2_{L^2(\Omega)}=\|u\|^2_{l^2}$,

$$\left\|\mathcal{I}_M U^{\varepsilon,n}\right\|_{L^2}=\left\|\mathcal{I}_M U^{\varepsilon,0}\right\|_{L^2},\quad n=1,2,\dots,N. \tag{4.35}$$

Before we derive the global error bounds, we introduce some usual notations and results. Similar to the case of unbounded domain, let

$$\mathbb{X}_M:=\mathrm{span}\left\{\varphi_l(x):-\frac{M}{2}\leq l\leq\frac{M}{2}-1\right\},$$

and define the tensor product $\mathbb{X}_M^d$ of d copies of $\mathbb{X}_M$ as

$$\mathbb{X}_M^d:=\mathbb{X}_M\otimes\cdots\otimes\mathbb{X}_M$$

with $\mathbb{X}_M^1=\mathbb{X}_M$. Let $\mathcal{P}_M:L^2(\Omega)\to\mathbb{X}_M^d$ be the L^2-orthogonal projection, defined by

$$(u-\mathcal{P}_M u,v)_{L^2(\Omega)}=0,\quad \forall v\in\mathbb{X}_M^d.$$

The following lemma bounds the error between $\mathcal{P}_M u$ and u.

Lemma 4.5 (see, e.g. [3,46]). *Suppose that $u\in H^r(\Omega)$ with $r>0$, then the following estimate holds:*

$$\|\mathcal{P}_M u-u\|_{L^2(\Omega)}\leq C_5 M^{-r}\|u\|_{H^r(\Omega)}. \tag{4.36}$$

The following lemma provides an upper bound for the error between the projection operator $\mathcal{P}_M$ and the interpolation operator $\mathcal{I}_M$.

Lemma 4.6 (see, e.g. [46]). *Suppose that $u\in H^r(\Omega)$ with $r>0$, then the following estimate holds:*

$$\|\mathcal{P}_M u-\mathcal{I}_M u\|_{L^2(\Omega)}\leq C_6 M^{-r}\|u\|_{H^r(\Omega)}. \tag{4.37}$$

4.2.2 Global error bounds for fully discrete approximation

Now following the idea and proof of [53], we have the following global error estimates.

Theorem 4.3 (Global Error Estimates)**.** *Let $u^\varepsilon = u^\varepsilon(x,t)$ be the analytic solution of* (1.1)*, and $U^{\varepsilon,n}$ be the discrete approximation given by* (4.29)-(4.30)*. Assume that the potential function $V \in C^2(\Omega)\cap H^{2s}(\Omega)$, and the solution $u^\varepsilon \in H^{4s}(\Omega)$. If*

$$\Delta t = \mathcal{O}(\varepsilon), \quad h = \mathcal{O}(\varepsilon), \tag{4.38}$$

then we have

$$\left\| u^\varepsilon(t_n) - \mathcal{I}_M U^{\varepsilon,n} \right\|_{L^2(\Omega)} \le C\left(\frac{\Delta t}{\varepsilon^2} + \frac{1}{(\varepsilon M)^{4s}}\right), \tag{4.39}$$

where C is independent of $\varepsilon, M, \Delta t$. Especially, if $\lambda \equiv 0$ (that is, the problem is linear), we have

$$\left\| u^\varepsilon(t_n) - \mathcal{I}_M U^{\varepsilon,n} \right\|_{L^2(\Omega)} \le C\left(\frac{\Delta t}{\varepsilon} + \frac{1}{(\varepsilon M)^{4s}}\right), \tag{4.40}$$

where C is also independent of $\varepsilon, M, \Delta t$.

We end this section with a few remarks about our results.

We first remark that to obtain a high accuracy numerical solution, we should choose Δt and M satisfying

$$\Delta t \le \varepsilon, \quad M > \frac{1}{\varepsilon}. \tag{4.41}$$

Under this condition, the Fourier-like spectral discretization will achieve spectral accuracy, independent of the fractional exponential s, provided that the analytic solution is sufficiently regular. This can be observed from the space convergence order $4s$, which depends on the space regularity of the analytic solution to (1.1), of numerical method in Theorems 4.1 and 4.3. We also observe from (4.39) that to obtain effective numerical solution one needs to choose $\Delta t < \varepsilon^{-2}$ since in this case the global error will be less than 1.

It is important to realize that the convergence orders of the fully discrete Lie-Trotter operator splitting methods with respect to the time step-size Δt is 1, independent of the fractional exponential s of Lalacian $(-\Delta)$, for both linear and nonlinear SDGPE.

The third remark is about the convergence order with respect to the critical parameter ε. When $\Delta t = \mathcal{O}(\varepsilon)$ and $h = \mathcal{O}(\varepsilon)$, the convergence order of the fully discrete Lie-Trotter operator splitting methods with respect to ε is -1 and -2 for both linear and nonlinear SDGPE, respectively. As pointed out in [12], however, this can not explain some numerical phenomena that the numerical convergence order of Lie-Trotter operator splitting method is $\mathcal{O}(\varepsilon^{-1})$ but not $\mathcal{O}(\varepsilon^{-2})$ with respect to the critical parameter ε when it was applied to some standard semiclassical NLS. For semiclassical nonlinear SDGPE, we observe these phenomena for several numerical examples but we also note that the error behaviour like $\mathcal{O}(\varepsilon^{-2})$ for a numerical examples involving the focusing nonlinearity (see numerical experiments in Section 5).

5 Numerical examples

We study here the convergence orders corresponding to the error estimates on several test cases. Let the convergence orders with respect to $\Delta t, h$, and ε be calculated by

$$\begin{aligned}&\mathrm{Order}_{\Delta t}=\log_2\left(E_\varepsilon^{2\Delta t,h}/E_\varepsilon^{\Delta t,h}\right),\\&\mathrm{Order}_h=\log_k\left(E_\varepsilon^{\Delta t,kh}/E_\varepsilon^{\Delta t,h}\right),\quad k>1,\\&\mathrm{Order}_\varepsilon=\log_2\left(E_{2\varepsilon}^{\Delta t,h}/E_\varepsilon^{\Delta t,h}\right),\end{aligned}$$

respectively, where $E_\varepsilon^{\Delta t,h}$ denotes the error $\|U^\varepsilon(t_n)-U^{\varepsilon,n}\|_{l^2}$ computed at $t=T$ with time step-size Δt and space step-size h for SDGPE (1.1) with Planck constant ε.

Example 5.1 (Semiclassical Sub-Diffusive NLS in Unbounded Domain)**.** We first consider applying Lie-Trotter operator splitting MCSG method to one-dimensional semiclassical sub-diffusive NLS (1.1)-(1.2) with $V\equiv 0$ in the unbounded domain. Let $T=0.5$ and

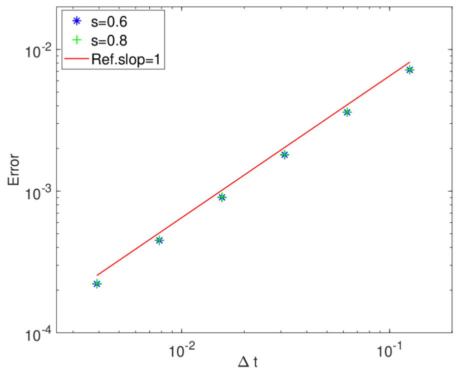
$$\sqrt{a_0(x)}=e^{-x^2},\quad \phi_0(x)=-\log\left(\exp(x)+\exp(-x)\right). \tag{5.1}$$

We consider two types of nonlinearity: focusing (repulsive) nonlinearity $\lambda=-1$, and defocusing (attractive) nonlinearity $\lambda=+1$.

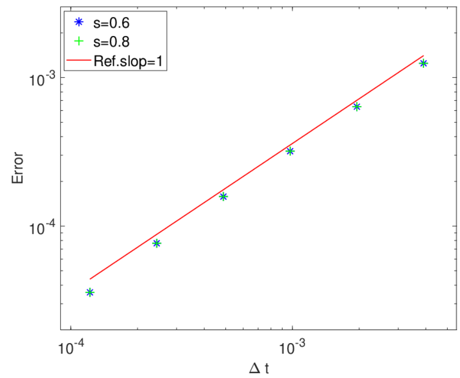
In the focusing case $\lambda=-1$, we first test the convergence order to the time step-size Δt and space step number M. For the case of $\varepsilon=2^{-3}$, we view the numerical solution obtained by using Lie-Trotter operator splitting MCSG method with $M=250$ and $\Delta t=2^{-13}$ as the reference solution. To observing the convergence order in time, we take $M=250$ and Δt varying from 2^{-3} to 2^{-8}. For the convergence order in space, we take $\Delta t=2^{-13}$ and M varying from 100 to 150. Moreover, we consider the case of $\varepsilon=2^{-7}$ and view the numerical solution by using Lie-Trotter operator splitting Fourier spectral method with $M=250$ and $\Delta t=2^{-16}$ as the reference solution. Similarity, we take $M=250$ and Δt varying from 2^{-8} to 2^{-13} to observe the convergence order in time, and $\Delta t=2^{-16}$ and M varying from 100 to 150 to observe the convergence order in space. From Figs. 1 and 2, we find the convergence order in time is order 1 and the convergence order in space is slightly large than $4s$, which is demonstrating the theoretical results in Theorem 4.3. It can be also observed from Fig. 2 that the smaller the fractional exponential s, the greater the errors, for both the cases of $\varepsilon=2^{-3}$ and $\varepsilon=2^{-7}$.

Now we consider the defocusing nonlinearity $\lambda=1$. We still consider two cases: $\varepsilon=2^{-3}$ and $\varepsilon=2^{-7}$ and perform the same computations as in the focusing nonlinearity $\lambda=-1$. All of numerical results presented in Figs. 3 and 4 demonstrate that the convergence orders of the Lie-Trotter splitting MCSG method for sub-diffusive NLS are consistent with the theoretical results in Theorem 4.3.

To show the numerically observed orders with respect to ε, we let ε vary from 2^{-2} to 2^{-8}. We views the numerical solution obtained by using Strang splitting MCSG method with $M=250$ and $\Delta t=2^{-16}$ as the reference solution. The errors between the reference

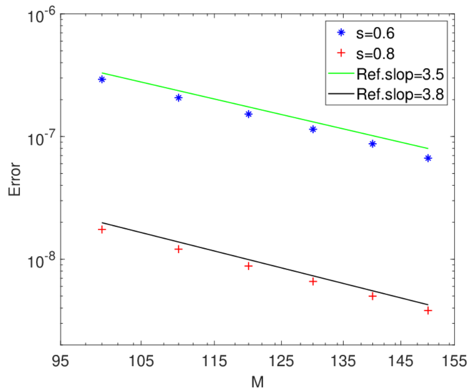


(a) Errors with respect to Δt, where $\varepsilon = 2^{-3}$

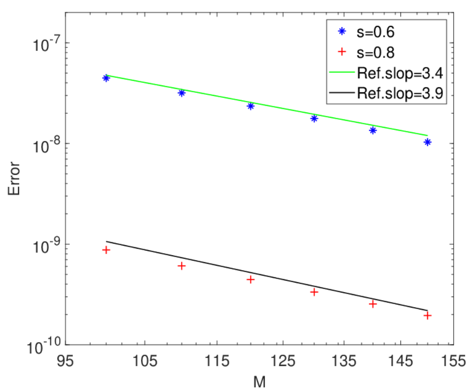


(b) Errors with respect to Δt, where $\varepsilon = 2^{-7}$

Figure 1: Errors of the Lie-Trotter splitting MCSG method for sub-diffusive NLS in the unbounded domain in Example 5.1 with $M = 250$ and $\lambda = -1$.

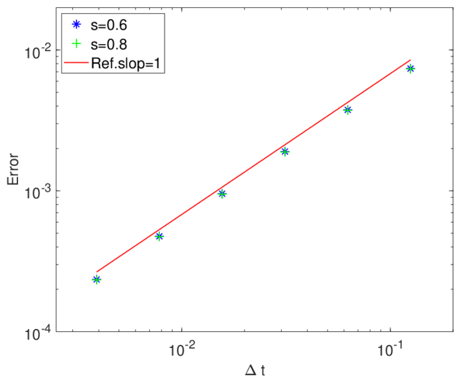


(a) Errors with respect to M, where $\varepsilon = 2^{-3}$

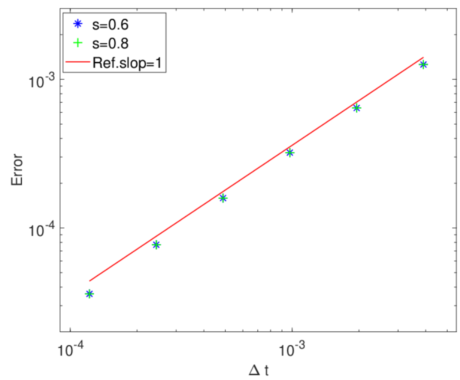


(b) Errors with respect to M, where $\varepsilon = 2^{-7}$

Figure 2: Errors of the Lie-Trotter splitting MCSG method for sub-diffusive NLS in unbounded domain in Example 5.1 with $\lambda = -1$.

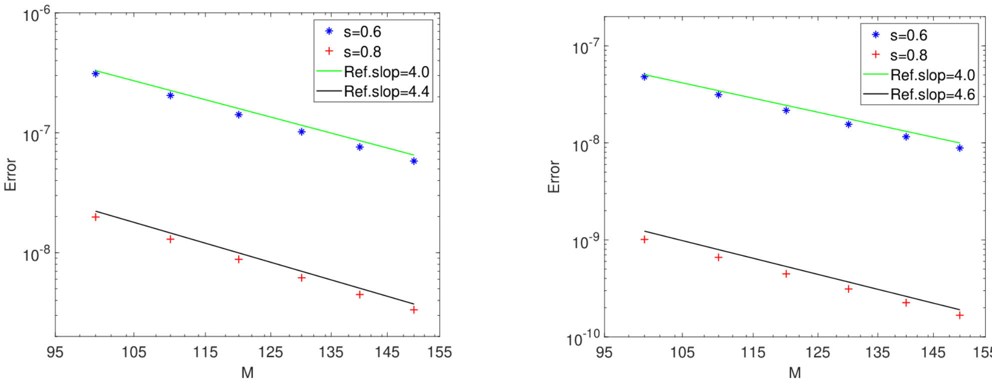


(a) Errors with respect to Δt, where $\varepsilon = 2^{-3}$



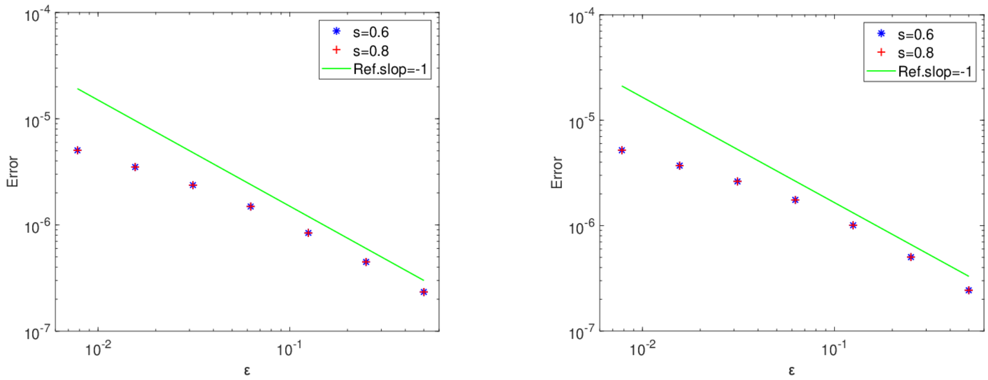
(b) Errors with respect to Δt, where $\varepsilon = 2^{-7}$

Figure 3: Errors of the Lie-Trotter splitting MCSG method for sub-diffusive NLS in the unbounded domain in Example 5.1 with $M = 250$ and $\lambda = 1$.



(a) Errors with respect to M, where $\varepsilon=2^{-3}$ (b) Errors with respect to M, where $\varepsilon=2^{-7}$

Figure 4: Errors of the Lie-Trotter splitting MCSG method for sub-diffusive NLS in the unbounded domain in Example 5.1 with $\lambda=1$.



(a) Errors with respect to ε, where $\lambda=-1$ (b) Errors with respect to ε, where $\lambda=1$

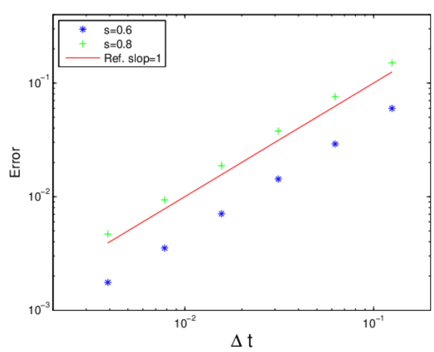
Figure 5: Errors of the LTSFS method for sub-diffusive NLS in Example 5.1 with $M=250$ and $\Delta t=2^{-16}$.

solution and the numerical solution computed by Lie-Trotter splitting MCSG method with $M=250$ and $\Delta t=2^{-16}$ are presented in Fig. 5. From these figure, it can be found that the convergence order with respect to ε is of order -1, independent of the fractional exponential s. This example illustrates that the theoretical analysis of numerical methods with respect to the Planck constant ε seems to be improved.

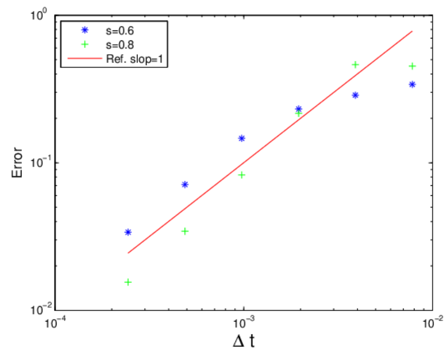
Example 5.2 (Semiclassical Sub-Diffusive NLS in Periodic Domain)**.** In the second experiment, we consider semiclassical sub-diffusive NLS (1.1)-(1.2) with periodic boundary condition $L=4$. In this case, we employ the Lie-Trotter splitting Fourier spectral (LTSFS) method to solve it. Let still $V\equiv 0, T=0.5$, and $a_0(x)$ and $\phi_0(x)$ be chosen as in (5.1).

In the focusing case $\lambda=-1$, we first test the convergence order with respect to the time step-size Δt. Let $\varepsilon=2^{-3}$. In this case, we view the numerical solution obtained by using Strang splitting Fourier spectral method with $h=2^{-13}$ and $\Delta t=2^{-13}$ as the reference solution. For numerical solution produced by the LTSFS method, we let $h=2^{-13}$, and let Δt vary from 2^{-3} to 2^{-8}. We also consider the case of $\varepsilon=2^{-7}$. In this case, we view the numerical solution by using Strang splitting Fourier spectral method with $h=2^{-13}$ and $\Delta t=2^{-15}$ as the reference solution. For numerical solution, we let $h=2^{-13}$, and let Δt vary from 2^{-7} to 2^{-12}. The numerical results are presented in Fig. 6 and further demonstrate that the LTSFS method is of order one with respect to Δt for both $\varepsilon=2^{-3}$ and $\varepsilon=2^{-7}$. We also observe from Fig. 5.2 that there is no attenuation behaviour for the errors of the LTSFS method when $\Delta t>\varepsilon$, that is, the condition $\Delta t\leq\varepsilon$ is necessary for the convergence of the LTSFS method.

To show numerically the convergence orders with respect to ε, we let ε vary from 2^{-3} to 2^{-8}. We still view the numerical solution by using Strang splitting Fourier spectral method with $h=2^{-13}$ and $\Delta t=2^{-13}$ as the reference solution. The errors between the reference solution and the numerical solution computed by LTSFS method with $h=2^{-13}$ and $\Delta t=2^{-13}$ are presented in Fig. 7. From this figure, we observe the convergence order of the LTSFS method is of order -2 with respect to ε, independent of the fractional exponential s. This is coincident with our theoretical findings in Theorem 4.3.



(a) Errors with respect to Δt, where $\varepsilon=2^{-3}$



(b) Errors with respect to Δt, where $\varepsilon=2^{-7}$

Figure 6: Errors of the LTSFS method with $h=2^{-13}$ for nonlinear SDGPE in Example 5.2: (a) $\varepsilon=2^{-3}$, (b) $\varepsilon=2^{-7}$.

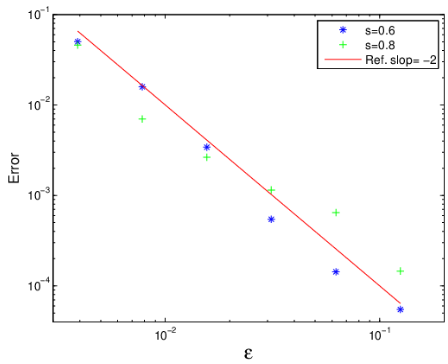
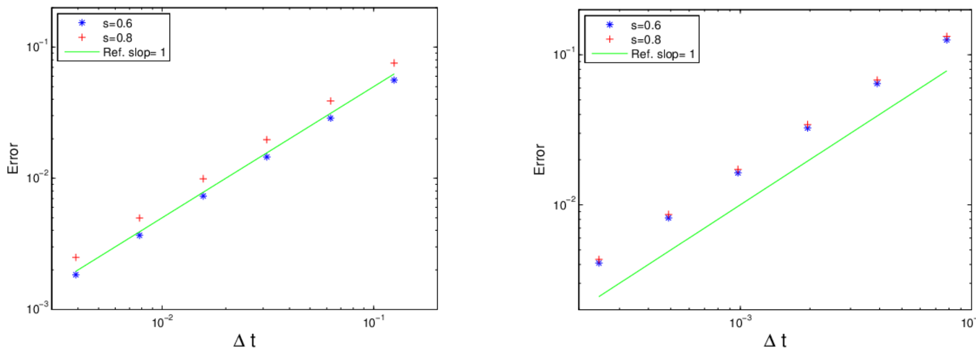


Figure 7: Errors of the LTSFS method for sub-diffusive NLS in Example 5.2, where $h=\Delta t=2^{-13}$, $\lambda=-1$.

Now we consider the defocusing nonlinearity $\lambda=1$. We still consider two cases: $\varepsilon=2^{-3}$ and $\varepsilon=2^{-7}$ and perform the same computations as in the focusing nonlinearity $\lambda=-1$. All of numerical results presented in Fig. 8 demonstrate that the convergence order of the LTSFS method with respect to Δt is 1, if the constraint (4.25) is satisfied.

When the small Planck constant vary from 2^{-3} to 2^{-8}, the errors between the reference solution and the numerical solution computed by the LTSFS method with $h=\Delta t=2^{-13}$ are presented in Fig. 9, from which we observe that the error bound provided in Theorem 4.3 is still valid. But the convergence order of the LTSFS method with respect to ε is larger than -2 and seem to be around -1. To clearly show the convergence order of the method, we also compute the cases $s=0.7$ and $s=0.9$ and list the numerical results in Table 1. From this table, we seem to be able to conjecture that the convergence order of the LTSFS method with respect to ε is -1 (the oscillation may arise from the coefficients C_2 in (3.24) or directly from the coefficients δ_i in priori estimates, since for different ε, the analytic solutions to SDGPE (1.1)-(1.2) are different and therefore the coefficients δ_i are different). This is also observed numerically for the case of $s=1$ in [12].



(a) Errors with respect to Δt, where $\varepsilon=2^{-3}$ (b) Errors with respect to Δt, where $\varepsilon=2^{-7}$

Figure 8: Errors of the LTSFS method for sub-diffusive NLS in Example 5.2, where $h=2^{-13},\lambda=1$.

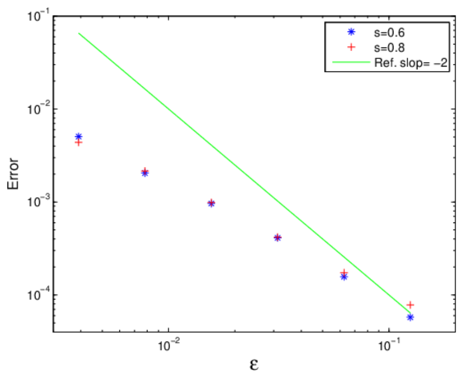


Figure 9: Errors of the LTSFS method for sub-diffusive NLS in Example 5.2, where $h=\Delta t=2^{-13}$, $\lambda=1$.

Table 1: The convergence orders Order_ε of LTSFS method with respect to ε in Example 5.2, where $h=\Delta t=2^{-13}$, $\lambda=1$.

ε	$s=0.6$	$s=0.7$	$s=0.8$	$s=0.9$
2^{-3}	–	–	–	–
2^{-4}	−1.4485	−1.2795	−1.1493	−0.9368
2^{-5}	−1.3883	−1.2812	−1.2681	−1.1797
2^{-6}	−1.2274	−1.1831	−1.2411	−1.3218
2^{-7}	−1.0843	−1.1831	−1.1272	−1.2637
2^{-8}	−1.3112	−0.9895	−1.0141	−1.1356

These imply that the numerical solution behaviour of the semiclassical sub-diffusive NLS is certainly much more complicated compared to the linear case (see the numerical results presented in [53] for linear case). On the one hand, this verifies our theoretical results, but on the other hand this is may be an indicator that the presented analysis can be improved for nonlinear case. We point out, though, that there is as yet no rigorous convergence result in the literature for the operator splitting spectral methods for the semiclassical sub-diffusive NLS. It is the first time that a rigorous error analysis is provided and numerically verified for the semiclassical sub-diffusive NLS.

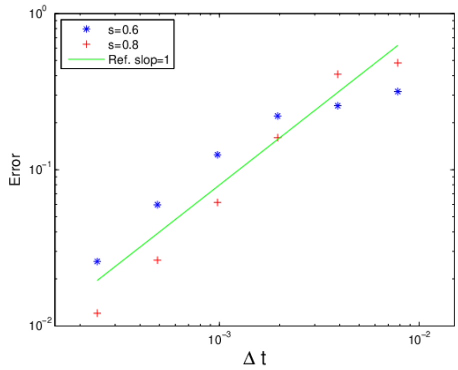
Example 5.3 (Semiclassical SDGPE with a Potential V)**.** In above two examples, the potential function V is set to be zero. In this example, we consider the effect of the electrostatic potential function V on the error behaviour of the numerical methods. For this purpose, we choose $V(x)=-x^2/2$ and initial datum as in Example 5.1. We let $T=0.5$. We still consider the periodic boundary condition but with $L=16$.

We first show the convergence order of the LTSFS method with respect to Δt. Since the smaller the parameter ε, the more difficult it is to solve the semiclassical SDGPE, we only consider the case of $\varepsilon=2^{-7}$ in this experiment. We let $h=2^{-11}$, which is smaller than ε, and let Δt vary from 2^{-7} to 2^{-12}. The errors are presented in Fig. 10 from which the correct order of convergence with respect to Δt is observed for both focusing nonlinearity $\lambda=-1$ and defocusing nonlinearity $\lambda=+1$.

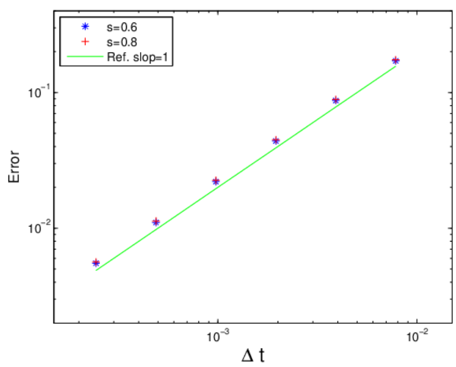
To demonstrate the convergence order of the LTSFS method with respect to ε, we let $h=2^{-11}$ and $\Delta t=2^{-13}$. The parameter ε varies from 2^{-3} to 2^{-8}. The numerical results are plotted in Fig. 11. The error behaviour of the LTSFS method for semiclassical SDGPE (1.1) with potential function $V=-x^2/2$ is the same as the method for semiclassical SDGPE with $V(x)\equiv 0$. This implies that the influence of the nonlinear term $\lambda|u^\varepsilon|^2u^\varepsilon$ in semiclassical SDGPE (1.1) on the error is stronger than that of linear term $V(x)$.

6 Concluding remarks

The SDGPE has been widely applied in the fields of science and engineering. In this work we studied the a priori estimates and numerical approximations of the solution

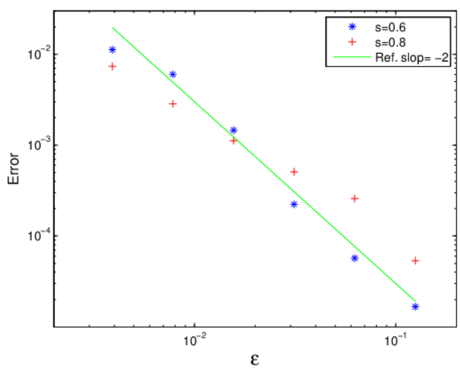


(a) Errors with respect to Δt, where $\lambda=-1$

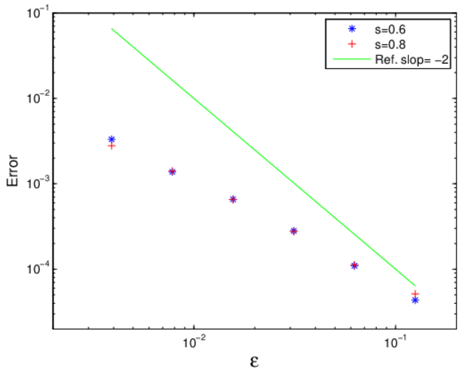


(b) Errors with respect to Δt, where $\lambda=1$

Figure 10: Errors of the LTSFS method for semiclassical SDGPE in Example 5.3, where $h=2^{-11}$ and $\varepsilon=2^{-7}$.



(a) Errors with respect to ε, where $\lambda=-1$



(b) Errors with respect to ε, where $\lambda=1$

Figure 11: Errors of the LTSFS method for semiclassical SDGPE in Example 5.3, where $h=2^{-11}$ and $\Delta t=2^{-13}$.

to semiclassical SDGPE (1.1), where the Planck constant ε is so small that it introduces difficulty in numerically solving such equation. We first established the a priori bounds for the solution to semiclassical SDGPE (1.1), which are fundamental in studying numerical error bounds. The local error bounds of Lie-Trotter operator splitting method for semiclassical SDGPE by using Lie commutator estimates of nonlinear operator. Based on these local error estimates, we derive the global error bounds for the fully discrete Lie-Trotter splitting MCSG method for the SDGPE in the unbounded domain and for the LTSFS approximation of the SDGPE with the periodic boundary condition. It was shown that the convergence order of both the numerical methods with respect to Δt is of order 1 independent of the fractional exponential s, and their convergence order with respect to the critical parameter ε is -1 and -2 for linear and nonlinear cases, respectively. To the best of our knowledge, this is the first paper where the theoretical analysis is made on the local and global error bounds of the operator splitting methods for semiclassical SDGPE, although the linear case has been investigated in [53].

We have implemented various numerical experiments for the two methods for semiclassical SDGPE (1.1), although there is no comparison between the numerical experiments and the exact physical experiments. For semiclassical SDGPE with focusing nonlinearity $\lambda=-1$, these numerical experiments exactly verify the theoretical results. The numerical results illustrate that our error estimates are also valid for semiclassical SDGPE with defocusing nonlinearity $\lambda=1$. Still, with the numerical observation in this paper and the numerical examples for standard Schrödinger equation ($s=1$) in the literature (see, e.g. [12] and their heuristic considerations), we conjecture that the convergence order of the LTSFS method with respect to the critical parameter ε for nonlinear SDGPE (1.1) with defocusing nonlinearity $\lambda=1$ is -1. This means that our results can be improved in this case and there exist different error behaviours with the Planck constant ε between the focusing and the defocusing nonlinearities. Studying these will be our future work.

It is well known that the Strang splitting method has higher convergence order than the Lie-Trotter splitting method. Extending the numerical analysis presented in this paper to the Strang splitting method will be another research work we are about to undertake.

Acknowledgments

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