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Error Analysis of the Strang Time-Splitting Laguerre–Hermite/Hermite Collocation Methods for the Gross–Pitaevskii Equation

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Abstract The aim of this paper is to carry out a rigorous error analysis for the Strang splitting Laguerre–Hermite/Hermite collocation methods for the time-dependent Gross–Pitaevskii equation (GPE). We derive error estimates for full discretizations of the three-dimensional GPE with cylindrical symmetry by the Strang splitting Laguerre–Hermite collocation method, and for the d-dimensional GPE by the Strang splitting Hermite collocation method.

Keywords Error analysis · Strang splitting · Laguerre and Hermite collocation method · Gross–Pitaevskii equation · Nonlinear Schrödinger equation

Mathematics Subject Classification 65D32 · 65N35 · 35J25

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1 Introduction

In this paper we consider the error analysis of fully discretized schemes for the Gross–Pitaevskii equation (GPE). The GPE, which is a nonlinear Schrödinger equation, describes Bose–Einstein condensates (BECs) in the low temperature regime (cf. [9, 19]):

$$\mathrm{i}\hbar\partial_t\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + NU_0\big|\psi(\mathbf{x},t)\big|^2\psi(\mathbf{x},t), \tag{1.1}$$

where ψ is the condensate wave function, m is the atomic mass, $\hbar$ is the Planck constant, N is the number of atoms in the condensate, and $V(\mathbf{x})$ is an external trapping potential. When a harmonic trap potential is considered, $V(\mathbf{x}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2)$, where ω_x, ω_y, and ω_z are the trap frequencies in the x-, y-, and z-directions, respectively. In most current experiments, the traps are cylindrically symmetric, i.e., $\omega_x = \omega_y$. $U_0 = \frac{4\pi\hbar^2 a_s}{m}$ describes the interaction between atoms in the condensate with the s-wave scattering length a_s (positive for repulsive interaction and negative for attractive interaction). Using the normalization

$$\int_{\mathbb{R}^3}\big|\psi(\mathbf{x},t)\big|^2\,\mathrm{d}\mathbf{x} = 1, \tag{1.2}$$

and denoting

$$V(\mathbf{x}) = \frac{1}{2}\big(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2\big), \quad \gamma_\alpha = \frac{\omega_\alpha}{\omega_m}, \ \alpha = x, y, z,$$

$$\omega_m = \min\{\omega_x, \omega_y, \omega_z\}, \qquad \beta = \frac{4\pi a_s N}{\sqrt{\hbar/m\omega_m}},$$

we arrive at the following dimensionless GPE:

$$\begin{cases} \mathrm{i}\partial_t\psi(\mathbf{x},t) = -\frac{1}{2}\Delta\psi(\mathbf{x},t) + V(\mathbf{x})\psi(\mathbf{x},t) + \beta|\psi(\mathbf{x},t)|^2\psi(\mathbf{x},t), \\ \psi(\mathbf{x},0) = \psi_0(\mathbf{x}), \qquad \lim_{|\mathbf{x}|\to\infty}\psi(\mathbf{x},t) = 0, \quad t \geq 0, \end{cases} \tag{1.3}$$

which is in fact a nonlinear Schrödinger equation.

Much attention has been devoted to numerical approximation of the time-dependent GPE (1.3). For instance, Bao, Jaksch and Markowich [2] and Bao and Shen [1] proposed several versions of time-splitting spectral methods, Ruprecht et al. [20] used the Crank–Nicolson finite difference method, and Cerimele et al. [5] proposed a particle-inspired scheme. However, the convergence analysis of semidiscretized Strang-type splitting schemes for linear and nonlinear Schrödinger equations only became available recently. Jahnke and Lubich [16] first presented an error bound for linear Schrödinger equations; then Lubich [18] gave an error bound for nonlinear Schrödinger equations. For related analyses in this direction, we refer to [6, 13, 17, 22]. However, to the authors' best knowledge, not much is available for the fully discretized time-splitting schemes for nonlinear Schrödinger equations. The main reason is that, unlike the error analysis for fully discrete non-splitting schemes (e.g., backward Euler or Crank–Nicolson schemes), the error analysis for fully discrete time-splitting schemes is much more difficult than that for their semidiscrete counterparts. Recently, Gauckler [8] performed an error analysis for a Hermite collocation Strang splitting method for the d-dimensional GPE. The aim of this paper is to carry out an error analysis for the Hermite–Laguerre collocation Strang splitting method for the three-dimensional GPE with cylindrical symmetry, and for the Hermite spectral Strang splitting method for the d-dimensional GPE.

Our main contributions are twofold: (i) our error analysis for the Hermite–Laguerre collocation method, which was actually implemented in [1], is new; (ii) our results for the Hermite collocation Strang splitting method for the d-dimensional GPE significantly improve the error estimates presented in [8]. Moreover, while our analysis for the semidiscretization in time is similar to those in [8, 18], our analysis for the full discretization has some essentially different components from those in [8], and leads to improved error estimates. Nevertheless, the techniques developed in [8, 18] have been very useful for our analysis.

More precisely, we first focus on the special case of (1.3) with cylindrical symmetry, i.e., $\gamma_x = \gamma_y = \gamma_r$ and $\psi_0(x, y, z) = \psi_0(r, z)$. Then the equation becomes:

$$\begin{cases} i\partial_t \psi(r,z,t) = [-\frac{1}{2r}\partial_r(r\partial_r\psi(r,z,t)) + \frac{1}{2}\gamma_r^2 r^2\psi(r,z,t)] \\ \qquad\qquad + [-\frac{1}{2}\partial_z^2\psi(r,z,t) + \frac{1}{2}\gamma_z^2 z^2\psi(r,z,t)] \\ \qquad\qquad + \beta|\psi(r,z,t)|^2\psi(r,z,t) =: \mathcal{A}_r\psi + \mathcal{B}_z\psi + \mathcal{N}(\psi), \\ \quad r \geq 0, z \in \mathbb{R}, \\ \psi(r,z,0) = \psi_0(r,z), \qquad \lim_{r,|z|\to\infty}\psi(r,z,t) = 0, \quad t \geq 0. \end{cases} \tag{1.4}$$

We present a full discretization scheme for (1.4) by using a Strang splitting scheme in time and a Laguerre–Hermite collocation method in space. The main results for (1.4) are summarized in Theorem 5.1 and Corollary 5.1. Note that the analysis for the axisymmetric case is much more difficult than the usual d-dimensional case due in part to the involvement of the Laguerre functions.

We then consider the full discretization of the d-dimensional GPE directly by using the Strang splitting in time and a Hermite collocation method in space. The main results for the d-dimensional GPE are summarized in Theorem 6.3 and Corollary 6.1.

The paper is organized as follows. In the next section, we derive some basic results for the Laguerre and Hermite approximations which will be used for the error analysis. In Sect. 3, we describe the semidiscrete Strang splitting scheme and the fully discrete Strang splitting Laguerre–Hermite collocation scheme for (1.4). The error analysis for the semidiscrete Strang splitting scheme for (1.4) is performed in Sect. 4, while that for the fully discrete Strang splitting Laguerre–Hermite collocation scheme is presented in Sect. 5. We consider the error analysis of the Strang splitting Hermite collocation scheme for the d-dimensional GPE in the last section.

2 Scaled Laguerre–Hermite–Gauss Interpolation

In this section, we describe scaled Laguerre–Hermite–Gauss interpolation and derive some basic results which will be used later.

2.1 Scaled Laguerre Functions

Let $I=(0,\infty)$ and let $L_m(\hat{r})$ be the Laguerre polynomial of degree m satisfying

$$\hat{r}L_m''(\hat{r})+(1-\hat{r})L_m'(\hat{r})+mL_m(\hat{r})=0,\quad \hat{r}\in I, m\geq 0,$$

$$\int_I L_m(\hat{r})L_n(\hat{r})\mathrm{e}^{-\hat{r}}\,\mathrm{d}\hat{r}=\delta_{mn},\quad m,n\geq 0,$$

where δ_{mn} is the Kronecker delta function.

For any positive integer N, we denote by $\mathcal{P}_N$ the set of all algebraic polynomials of degree at most N. Let $\{\hat{r}_j,\hat{\omega}_j^r\}_{j=0}^N$ be the Laguerre–Gauss points and weights, and $\hat{\mathcal{I}}_N^r: C(I)\to\mathcal{P}_N$ be the corresponding interpolation operator in the r-direction such that

$$\hat{\mathcal{I}}_N^r v(\hat{r}_j)=v(\hat{r}_j),\quad 0\leq j\leq N.$$

For any integer $r\geq 0$, we define the weighted Sobolev space $H_\chi^r(I)$ with the weight function χ in the usual way. In particular, $L_\chi^2(I)=H_\chi^0(I)$. For any $r>0$, we define the space $H_\chi^r(I)$ by space interpolation as in [4]. According to Theorem 3.4 of [11], for any $v\in H_{\omega_0}^1(I)$ and $\partial_{\hat{r}}v\in L_{\omega_1}^2(I)$ with $\omega_0(\hat{r})=\mathrm{e}^{-\hat{r}}$ and $\omega_1(\hat{r})=\hat{r}\mathrm{e}^{-\hat{r}}$, we have

$$\|\hat{\mathcal{I}}_N^r v\|_{L_{\omega_0}^2(I)}\leq cN^{-\frac{1}{2}}\|\partial_{\hat{r}}v\|_{L_{\omega_0}^2(I)}+c(\ln N)^{\frac{1}{2}}\big(\|v\|_{L_{\omega_0}^2(I)}+\|\partial_{\hat{r}}v\|_{L_{\omega_1}^2(I)}\big).\tag{2.1}$$

In order to determine the eigenfunctions of the linear operators $\mathcal{A}_r$, Bao and Shen [1] introduced the change of variable $r=\sqrt{\frac{\hat{r}}{\gamma_r}}$ and the scaled Laguerre function

$$l_m(r)=\sqrt{\frac{\gamma_r}{\pi}}\mathrm{e}^{-\hat{r}/2}L_m(\hat{r})=\sqrt{\frac{\gamma_r}{\pi}}\mathrm{e}^{-\gamma_r r^2/2}L_m\big(\gamma_r r^2\big),\quad r\in I,\tag{2.2}$$

which satisfies

$$\begin{aligned}&\mathcal{A}_r l_m(r):=-\frac{1}{2r}\partial_r\big(r\partial_r l_m(r)\big)+\frac{1}{2}\gamma_r^2 r^2 l_m(r)=\mu_m^r l_m(r),\\&\mu_m^r=\gamma_r(2m+1), m\geq 0,\end{aligned}\tag{2.3}$$

$$2\pi\int_I l_m(r)l_n(r)r\,\mathrm{d}r=\delta_{mn},\quad m,n\geq 0.\tag{2.4}$$

We also denote

$$r_j=\sqrt{\frac{\hat{r}_j}{\gamma_r}},\qquad \omega_j^r=\frac{\pi}{\gamma_r}\hat{\omega}_j^r\mathrm{e}^{\hat{r}_j},\qquad X_N^r=\mathrm{span}\big\{l_m(r):0\leq m\leq N\big\},$$

where r_j and ω_j^r are the scaled Laguerre–Gauss points and weights, respectively. We recall that [1]:

$$\sum_{j=0}^{N} \omega_j^r l_m(r_j) l_n(r_j) = \delta_{nm}, \quad \forall 0 \le n+m \le 2N+1. \tag{2.5}$$

Next, we define $\mathcal{I}_N^r : C(I) \to X_N^r$, the corresponding interpolation operator, by

$$\mathcal{I}_N^r u(r_j) = u(r_j), \quad 0 \le j \le N.$$

For any $u(r) = \mathrm{e}^{-\gamma_r r^2/2} v(\gamma_r r^2)$, we have

$$\mathrm{e}^{\gamma_r r_j^2/2} \mathcal{I}_N^r u(r_j) = \mathrm{e}^{\gamma_r r_j^2/2} u(r_j) = v(\hat{r}_j) = \hat{\mathcal{I}}_N^r v(\hat{r}_j), \quad 0 \le j \le N.$$

Furthermore, due to (2.2), $\mathrm{e}^{\gamma_r r^2/2} \mathcal{I}_N^r u(r)\big|_{r=\sqrt{\frac{\hat{r}}{\gamma_r}}} \in \mathcal{P}_N$ and $\hat{\mathcal{I}}_N^r v(\hat{r}) \in \mathcal{P}_N$. Hence,

$$\mathrm{e}^{\gamma_r r^2/2} \mathcal{I}_N^r u(r)\big|_{r=\sqrt{\frac{\hat{r}}{\gamma_r}}} = \hat{\mathcal{I}}_N^r v(\hat{r}).$$

This with (2.1) leads to

$$\begin{aligned}
\int_I \left|\mathcal{I}_N^r u\right|^2 r \,\mathrm{d}r &\le cN^{-1}\left(\int_I \left|u(r)\right|^2 r \,\mathrm{d}r + \int_I \left|\partial_r u(r)\right|^2 r^{-1} \,\mathrm{d}r\right) \\
&\quad + c\ln N\left(\int_I \left|u(r)\right|^2 \left(r + r^3\right) \mathrm{d}r + \int_I \left|\partial_r u(r)\right|^2 r \,\mathrm{d}r\right) \\
&\le cN^{-1} \int_I \left|\partial_r u(r)\right|^2 r^{-1} \,\mathrm{d}r + c\ln N\left(\int_I \left|u(r)\right|^2 \left(r + r^3\right) \mathrm{d}r\right. \\
&\quad \left. + \int_I \left|\partial_r u(r)\right|^2 r \,\mathrm{d}r\right).
\end{aligned} \tag{2.6}$$

2.2 Scaled Hermite Functions

Let $H_l(z)$ be the standard Hermite polynomials satisfying

$$H_l''(z) - 2z H_l'(z) + 2l H_l(z) = 0, \quad z \in \mathbb{R}, l \ge 0,$$

$$\int_{\mathbb{R}} H_l(z) H_n(z) \mathrm{e}^{-z^2} \,\mathrm{d}z = \sqrt{\pi} 2^l l! \delta_{ln}, \quad l, n \ge 0.$$

We consider the scaled Hermite function (cf. [1])

$$h_l(z) = (\gamma_z/\pi)^{\frac{1}{4}} \mathrm{e}^{-\gamma_z z^2/2} H_l(\sqrt{\gamma_z} z)/\sqrt{2^l l!}, \quad z \in \mathbb{R}, \tag{2.7}$$

which satisfies

$$\mathcal{B}_z h_l(z) := -\frac{1}{2} h_l''(z) + \frac{1}{2}\gamma_z^2 z^2 h_l(z) = \mu_l^z h_l(z), \quad \mu_l^z = \frac{2l+1}{2}\gamma_z, l \ge 0, \tag{2.8}$$

$$\int_{\mathbb{R}} h_l(z)h_n(z)\,\mathrm{d}z = \delta_{ln}, \quad l,n \geq 0. \tag{2.9}$$

Next let $\{\hat{z}_k, \hat{\omega}_k^z\}_{k=0}^N$ be the Hermite–Gauss points and weights. Denote by

$$z_k = \frac{\hat{z}_k}{\sqrt{\gamma_z}}, \qquad \omega_k^z = \frac{\hat{\omega}_k^z}{\sqrt{\gamma_z}}\mathrm{e}^{\hat{z}_k^2},$$

the scaled Hermite–Gauss points and weights, respectively. According to [1],

$$\sum_{k=0}^N \omega_k^z h_m(z_k)h_n(z_k) = \delta_{nm}, \quad \forall 0 \leq n+m \leq 2N+1. \tag{2.10}$$

Let $X_N^z = \operatorname{span}\{h_l(z) : 0 \leq l \leq N\}$. We define the scaled Hermite–Gauss interpolation operator $\mathcal{I}_N^z : C(\mathbb{R}) \to X_N^z$ by

$$\mathcal{I}_N^z v(z_k) = v(z_k), \quad 0 \leq k \leq N.$$

The following result is established in [10]:

$$\left\|\mathcal{I}_N^z v\right\|_{L^2(\mathbb{R})} \leq c\big(\|v\|_{L^2(\mathbb{R})} + N^{-\frac{1}{6}}|v|_{H^1(\mathbb{R})}\big), \quad v \in H^1(\mathbb{R}), \tag{2.11}$$

where $|\cdot|_{H^1(\mathbb{R})}$ denotes the seminorm of $H^1(\mathbb{R})$.

We now introduce some properties about the scaled Hermite functions in $\mathbb{R}^3$. Let $h_k(x)$ and $h_m(y)$ be the Hermite functions defined in (2.7) with γ_x and γ_y instead of γ_z, respectively. The corresponding operators in (2.8) are denoted by $\mathcal{B}_x$ and $\mathcal{B}_y$, respectively, i.e.,

$$\mathcal{B}_x h_k(x) := -\frac{1}{2}h_k''(x) + \frac{1}{2}\gamma_x^2 x^2 h_k(x) = \mu_k^x h_k(x), \quad \mu_k^x = \frac{2k+1}{2}\gamma_x, \tag{2.12}$$

$$\mathcal{B}_y h_m(y) := -\frac{1}{2}h_m''(y) + \frac{1}{2}\gamma_y^2 y^2 h_m(y) = \mu_m^y h_m(y), \quad \mu_m^y = \frac{2m+1}{2}\gamma_y. \tag{2.13}$$

We denote by $L^2(\mathbb{R}^3)$ and $H^s(\mathbb{R}^3)$ $(s > 0)$ the usual Sobolev spaces with the usual notation for their seminorms and norms. It can be easily shown that the linear differential operator $\mathcal{B}_x + \mathcal{B}_y + \mathcal{B}_z$ is positive definite and self-adjoint. Indeed, for any u and v in the domain of $\mathcal{B}_x + \mathcal{B}_y + \mathcal{B}_z$, applying integration by parts leads to

$$\begin{aligned} \big((\mathcal{B}_x + \mathcal{B}_y + \mathcal{B}_z)u, v\big)_{\mathbb{R}^3} = \big(u, (\mathcal{B}_x + \mathcal{B}_y + \mathcal{B}_z)v\big)_{\mathbb{R}^3} = a(u,v), \\ \big((\mathcal{B}_x + \mathcal{B}_y + \mathcal{B}_z)u, u\big)_{\mathbb{R}^3} = a(u,u) > 0, \quad \text{if } u \neq 0, \end{aligned} \tag{2.14}$$

where

$$a(u,v) = \frac{1}{2}(\nabla u, \nabla v)_{\mathbb{R}^3} + \frac{1}{2}\big(\big(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2\big)u, v\big)_{\mathbb{R}^3}.$$

From (2.8), (2.9), (2.12), and (2.13), we have

$$
\begin{aligned}
&a\big(h_k(x)h_m(y)h_l(z), h_{k'}(x)h_{m'}(y)h_{l'}(z)\big) \\
&\quad = \big((\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)h_k(x)h_m(y)h_l(z), h_{k'}(x)h_{m'}(y)h_{l'}(z)\big)_{\mathbb{R}^3} \\
&\quad = \big(\mu_k^x+\mu_m^y+\mu_l^z\big)\delta_{kk'}\delta_{mm'}\delta_{ll'}. \qquad (2.15)
\end{aligned}
$$

Since $\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z$ is a positive definite and self-adjoint operator in $L^2(\mathbb{R}^3)$, the fractional power $(\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^{1/2}$ is well defined, and the associated norms can be characterized by (see, e.g., [21, 23]):

$$
\big\|(\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^{1/2}u\big\|^2_{L^2(\mathbb{R}^3)} = a(u,u), \qquad (2.16)
$$

$$
\big\|(\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^{m+1/2}u\big\|^2_{L^2(\mathbb{R}^3)} = a\big((\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^m u, (\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^m u\big), \quad \forall m\in\mathbb{N}. \qquad (2.17)
$$

For any $u\in L^2(\mathbb{R}^3)$, we write (cf. [8])

$$
u(x,y,z) = \sum_{k,m,l=0}^{\infty} u_{kml}h_k(x)h_m(y)h_l(z).
$$

We introduce the following three Sobolev spaces equipped with the norms:

$$
\begin{aligned}
\|u\|_{H_A^s(\mathbb{R}^3)} &= \left(\sum_{k,m,l=0}^{\infty}\big(\mu_k^x+\mu_m^y+\mu_l^z\big)^s|u_{kml}|^2\right)^{\frac{1}{2}}, \\
\|u\|_{H_B^s(\mathbb{R}^3)} &= \big\|(\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^{\frac{s}{2}}u\big\|_{L^2(\mathbb{R}^3)}, \\
\|u\|_{H_C^s(\mathbb{R}^3)} &= \left(\sum_{k+m+l=0}^{s}\big\|\big(x^2+y^2+z^2+1\big)^{\frac{s-k-m-l}{2}}\partial_x^k\partial_y^m\partial_z^l u\big\|^2_{L^2(\mathbb{R}^3)}\right)^{\frac{1}{2}}.
\end{aligned}
$$

With a slight modification of Lemma 2.1 in [25], we can prove the following.

Lemma 2.1 *The previous three norms are equivalent, i.e.,*

$$
\|u\|_{H_A^s(\mathbb{R}^3)} = \|u\|_{H_B^s(\mathbb{R}^3)} \sim \|u\|_{H_C^s(\mathbb{R}^3)}.
$$

Proof Let integer $r\geq 0$. According to (2.8), (2.9), (2.12), and (2.13), we have that for $s=2r$,

$$
\begin{aligned}
\|u\|^2_{H_B^s(\mathbb{R}^3)} &= \big((\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^r u, (\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^r u\big)_{\mathbb{R}^3} \\
&= \left(\sum_{k,m,l=0}^{\infty}\big(\mu_k^x+\mu_m^y+\mu_l^z\big)^r u_{kml}h_kh_mh_l,\right.
\end{aligned}
$$

$$\left.\sum_{k',m',l'=0}^{\infty}\left(\mu_{k'}^x+\mu_{m'}^y+\mu_{l'}^z\right)^r u_{k'm'l'}h_{k'}h_{m'}h_{l'}\right)_{\mathbb{R}^3}$$

$$=\sum_{k,m,l=0}^{\infty}\left(\mu_k^x+\mu_m^y+\mu_l^z\right)^{2r}|u_{kml}|^2=\|u\|^2_{H_A^s(\mathbb{R}^3)}.$$

Next, by (2.15) and (2.17), we deduce that for $s=2r+1$,

$$\begin{aligned}\|u\|^2_{H_B^s(\mathbb{R}^3)} &= a\big((\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^r u,(\mathcal{B}_x+\mathcal{B}_y+\mathcal{B}_z)^r u\big)\\ &= a\left(\sum_{k,m,l=0}^{\infty}\left(\mu_k^x+\mu_m^y+\mu_l^z\right)^r u_{kml}h_kh_mh_l,\right.\\ &\qquad\left.\sum_{k',m',l'=0}^{\infty}\left(\mu_{k'}^x+\mu_{m'}^y+\mu_{l'}^z\right)^r u_{k'm'l'}h_{k'}h_{m'}h_{l'}\right)\\ &= \sum_{k,m,l,k',m',l'=0}^{\infty}\left(\mu_k^x+\mu_m^y+\mu_l^z\right)^r\left(\mu_{k'}^x+\mu_{m'}^y+\mu_{l'}^z\right)^r\\ &\qquad\times u_{kml}\overline{u}_{k'm'l'}a(h_kh_mh_l,h_{k'}h_{m'}h_{l'})\\ &= \sum_{k,m,l=0}^{\infty}\left(\mu_k^x+\mu_m^y+\mu_l^z\right)^{2r+1}|u_{kml}|^2=\|u\|^2_{H_A^s(\mathbb{R}^3)}.\end{aligned}$$

The above two estimates, together with function space interpolation as in [4], lead to the desired result $\|u\|_{H_A^s(\mathbb{R}^3)}=\|u\|_{H_B^s(\mathbb{R}^3)}$. Furthermore, following [25] we can verify readily that

$$\|u\|_{H_A^s(\mathbb{R}^3)}\sim\|u\|_{H_C^s(\mathbb{R}^3)}.$$

This completes the proof. □

Remark 2.1 We note that Helffer [14] proved the following equivalence result:

$$\begin{aligned}&\|u\|_{L^2(\mathbb{R}^3)}+\left\|(\mathcal{B}_x+\mathcal{B}_y)^{\frac{s}{2}}u\right\|_{L^2(\mathbb{R}^3)}+\left\|\mathcal{B}_z^{\frac{s}{2}}u\right\|_{L^2(\mathbb{R}^3)}\\ &\quad\sim\|u\|_{H^s(\mathbb{R}^3)}+\left\|\left(x^2+y^2\right)^{\frac{s}{2}}u\right\|_{L^2(\mathbb{R}^3)}+\left\|z^s u\right\|_{L^2(\mathbb{R}^3)}.\end{aligned}$$

The above result, although very similar to Lemma 2.1, is nevertheless different. Furthermore, Abdallah, Castella, and Méhats [3] extended the above result to the more general case with nonharmonic oscillator.

Lemma 2.2 *We have the following inequalities*:

$$\|uvw\|_{L^2(\mathbb{R}^3)}\le c\|u\|_{H^1(\mathbb{R}^3)}\|v\|_{H^1(\mathbb{R}^3)}\|w\|_{H^1(\mathbb{R}^3)}, \tag{2.18}$$

$$\|uvw\|_{L^2(\mathbb{R}^3)}\le c\|u\|_{L^2(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)}, \tag{2.19}$$

$$\|uvw\|_{H^1(\mathbb{R}^3)} \le c\|u\|_{H^1(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)}, \tag{2.20}$$

$$\|uvw\|_{H^k(\mathbb{R}^3)} \le c\|u\|_{H^k(\mathbb{R}^3)}\|v\|_{H^k(\mathbb{R}^3)}\|w\|_{H^k(\mathbb{R}^3)}, \quad \forall \text{ integer } k \ge 2. \tag{2.21}$$

Proof The results (2.18)–(2.20) and (2.21) with $k=2$ are established in [18]. By induction, we can obtain the result (2.21) with integer $k \ge 3$. □

The previous results can be extended to the corresponding ones in $H^s_A(\mathbb{R}^3)$, as stated below.

Lemma 2.3 *The following inequalities hold*:

$$\|uvw\|_{L^2(\mathbb{R}^3)} \le c\|u\|_{H^1_A(\mathbb{R}^3)}\|v\|_{H^1_A(\mathbb{R}^3)}\|w\|_{H^1_A(\mathbb{R}^3)}. \tag{2.22}$$

$$\|uvw\|_{L^2(\mathbb{R}^3)} \le c\|u\|_{L^2(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}. \tag{2.23}$$

$$\|uvw\|_{H^1_A(\mathbb{R}^3)} \le c\|u\|_{H^1_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}. \tag{2.24}$$

$$\|uvw\|_{H^k_A(\mathbb{R}^3)} \le c\|u\|_{H^k_A(\mathbb{R}^3)}\|v\|_{H^k_A(\mathbb{R}^3)}\|w\|_{H^k_A(\mathbb{R}^3)}, \quad \forall \text{ integer } k \ge 2. \tag{2.25}$$

Proof Cases 1 and 2. Since $\|u\|_{H^s_A(\mathbb{R}^3)} \sim \|u\|_{H^s_C(\mathbb{R}^3)}$, we have $\|u\|_{H^s(\mathbb{R}^3)} \le c\|u\|_{H^s_A(\mathbb{R}^3)}$, $s \ge 0$. Hence by (2.18) and (2.19) we get the results (2.22) and (2.23).

Case 3. According to the equivalence of the norms, we derive readily that

$$\|uvw\|_{H^1_A(\mathbb{R}^3)} \le c\|uvw\|_{H^1_C(\mathbb{R}^3)} \le c|uvw|_{H^1(\mathbb{R}^3)} + c\left\|\left(x^2+y^2+z^2+1\right)^{\frac{1}{2}} uvw\right\|_{L^2(\mathbb{R}^3)}.$$

From (2.20) we have

$$|uvw|_{H^1(\mathbb{R}^3)} \le c\|u\|_{H^1(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)} \le c\|u\|_{H^1_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}.$$

By (2.19),

$$\begin{aligned}
&\left\|\left(x^2+y^2+z^2+1\right)^{\frac{1}{2}} uvw\right\|_{L^2(\mathbb{R}^3)} \\
&\quad \le c\left\|\left(x^2+y^2+z^2+1\right)^{\frac{1}{2}} u\right\|_{L^2(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)} \\
&\quad \le c\|u\|_{H^1_C(\mathbb{R}^3)}\|v\|_{H^2_C(\mathbb{R}^3)}\|w\|_{H^2_C(\mathbb{R}^3)} \\
&\quad \le c\|u\|_{H^1_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}.
\end{aligned} \tag{2.26}$$

A combination of the previous three inequalities leads to the desired result (2.24).

Case 4. Obviously,

$$\begin{aligned}
\|uvw\|_{H^2_A(\mathbb{R}^3)} &\le c|uvw|_{H^2(\mathbb{R}^3)} \\
&\quad + c\sum_{k+m+l=1}\left\|\left(x^2+y^2+z^2+1\right)^{\frac{1}{2}}\partial_x^k\partial_y^m\partial_z^l(uvw)\right\|_{L^2(\mathbb{R}^3)} \\
&\quad + c\left\|\left(x^2+y^2+z^2+1\right)uvw\right\|_{L^2(\mathbb{R}^3)}.
\end{aligned}$$

From (2.21),

$$|uvw|_{H^2(\mathbb{R}^3)} \le c\|u\|_{H^2(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)} \le c\|u\|_{H^2_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}.$$

Since $\|(x^2+y^2+z^2+1)^{\frac{1}{2}}\partial_x u\|_{L^2(\mathbb{R}^3)} \le \|u\|_{H^2_C(\mathbb{R}^3)}$, we can use an argument similar to (2.26) to derive that

$$\begin{aligned}
\sum_{k+m+l=1} &\big\|\big(x^2+y^2+z^2+1\big)^{\frac{1}{2}}\partial_x^k\partial_y^m\partial_z^l(uvw)\big\|_{L^2(\mathbb{R}^3)} \\
&\le c\|u\|_{H^2_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}.
\end{aligned}$$

Furthermore, by (2.19),

$$\begin{aligned}
&\big\|\big(x^2+y^2+z^2+1\big)uvw\big\|_{L^2(\mathbb{R}^3)} \\
&\quad\le c\big\|\big(x^2+y^2+z^2+1\big)u\big\|_{L^2(\mathbb{R}^3)}\|v\|_{H^2(\mathbb{R}^3)}\|w\|_{H^2(\mathbb{R}^3)} \\
&\quad\le c\|u\|_{H^2_A(\mathbb{R}^3)}\|v\|_{H^2_A(\mathbb{R}^3)}\|w\|_{H^2_A(\mathbb{R}^3)}.
\end{aligned}$$

Therefore, a combination of the previous four inequalities leads to (2.25) with $k=2$. We can obtain the desired results for integer $k \ge 3$ by using an argument as in the proof of (6.14) of this paper. □

2.3 Approximation by the Mixed Laguerre–Hermite Functions

Set $\Omega = I \times \mathbb{R}$. In order to present the convergence of the three-dimensional GPE with cylindrical symmetry, we need some approximation results on the mixed Laguerre–Hermite functions. To this end, we define the inner product and norm of $L^2(\Omega)$ with complex-valued functions by

$$(u,v)_\Omega = 2\pi\int_\Omega u(r,z)\overline{v}(r,z)r\,\mathrm{d}r\,\mathrm{d}z, \qquad \|v\|_{L^2(\Omega)} = (v,v)_\Omega^{\frac{1}{2}}.$$

We notice that the inner product introduced here is not the usual inner product on $L^2(I\times\mathbb{R})$, but on $L^2(\mathbb{R}^3)$ using cylindrical coordinates. For any $u(r,z) \in L^2(\Omega)$, we write

$$u(r,z) = \sum_{m,l=0}^{\infty} u_{ml}l_m(r)h_l(z).$$

Obviously, the linear differential operator $\mathcal{A}_r + \mathcal{B}_z$ is positive definite and self-adjoint. Thus for any u and v in the domain of $\mathcal{A}_r+\mathcal{B}_z$,

$$\begin{aligned}
&\big((\mathcal{A}_r+\mathcal{B}_z)u,v\big)_\Omega = \big(u,(\mathcal{A}_r+\mathcal{B}_z)v\big)_\Omega = b(u,v), \\
&\big((\mathcal{A}_r+\mathcal{B}_z)u,u\big)_\Omega = b(u,u) > 0, \quad \text{if } u \ne 0,
\end{aligned} \tag{2.27}$$

where the bilinear form

$$b(u,v) = \frac{1}{2}(\nabla u,\nabla v)_\Omega + \frac{1}{2}\big(\big(\gamma_r^2r^2+\gamma_z^2z^2\big)u,v\big)_\Omega.$$

Moreover, for any functions $l_m(r)h_l(z)$ and $l_{m'}(r)h_{l'}(z)$,

$$b(l_m h_l, l_{m'} h_{l'}) = \big((\mathcal{A}_r + \mathcal{B}_z) l_m h_l, l_{m'} h_{l'}\big)_\Omega = \big(\mu_m^r + \mu_l^z\big)\delta_{mm'}\delta_{ll'}. \tag{2.28}$$

The fractional power $(\mathcal{A}_r + \mathcal{B}_z)^{1/2}$ is also well defined, and the associated norms can be characterized by

$$\big\|(\mathcal{A}_r + \mathcal{B}_z)^{1/2} u\big\|_\Omega^2 = b(u, u), \tag{2.29}$$

$$\big\|(\mathcal{A}_r + \mathcal{B}_z)^{m+1/2} u\big\|_\Omega^2 = b\big((\mathcal{A}_r + \mathcal{B}_z)^m u, (\mathcal{A}_r + \mathcal{B}_z)^m u\big), \quad \forall m \in \mathbb{N}. \tag{2.30}$$

We next introduce two Sobolev spaces equipped with the norms:

$$\|u\|_{H_A^s(\Omega)} = \left(\sum_{m,l=0}^{\infty} \big(\mu_m^r + \mu_l^z\big)^s |u_{ml}|^2\right)^{\frac{1}{2}},$$

$$\|u\|_{H_B^s(\Omega)} = \big\|(\mathcal{A}_r + \mathcal{B}_z)^{\frac{s}{2}} u\big\|_{L^2(\Omega)}.$$

It is also easy to verify that $\|u\|_{H_A^s(\Omega)} = \|u\|_{H_B^s(\Omega)}$.

Let $X_N := X_N(\gamma_r, \gamma_z) = \text{span}\{l_m(r)h_l(z) : 0 \le m, l \le N\}$. According to (2.3) and (2.8), $\{l_m(r)h_l(z)\}$ are the eigenfunctions of the operator $\mathcal{A}_r + \mathcal{B}_z$ with the eigenvalues $\mu_m^r + \mu_l^z$.

Lemma 2.4 *For any $\phi \in X_N$ and $s \ge 0$,*

$$\|\phi\|_{H_A^s(\Omega)} \le c N^{\frac{s}{2}} \|\phi\|_{L^2(\Omega)}.$$

Proof Given $\phi \in X_N$, we write

$$\phi(r, z) = \sum_{m,l=0}^{N} \phi_{ml} l_m(r) h_l(z).$$

For any integer $s \ge 0$,

$$\|\phi\|_{H_A^s(\Omega)}^2 = \big((\mathcal{A}_r + \mathcal{B}_z)^s \phi, \phi\big)_\Omega = \sum_{m,l=0}^{N} \big(\mu_m^r + \mu_l^z\big)^s |\phi_{ml}|^2$$

$$\le c N^s \sum_{m,l=0}^{N} |\phi_{ml}|^2 = c N^s \|\phi\|_{L^2(\Omega)}^2.$$

This with a standard space interpolation technique [4] yields the desired result. □

We now consider the orthogonal projection. For any $u \in L^2(\Omega)$, the orthogonal projection operator $P_N : L^2(\Omega) \to X_N$ is defined by

$$(u - P_N u, \phi)_\Omega = 0, \quad \forall \phi \in X_N. \tag{2.31}$$

In particular, if $u \in H_B^s(\Omega)$ with integer $s \ge 0$, we have

$$\begin{aligned}&\big((\mathcal{A}_r+\mathcal{B}_z)^{\frac{s}{2}}(u-P_N u),(\mathcal{A}_r+\mathcal{B}_z)^{\frac{s}{2}}\phi\big)_\Omega\\&\quad=\big(u-P_N u,(\mathcal{A}_r+\mathcal{B}_z)^s\phi\big)_\Omega=0,\quad \forall\phi\in X_N,\end{aligned}\tag{2.32}$$

which means that the $L^2(\Omega)$-orthogonal projection operator P_N is also the $H_B^s(\Omega)$-orthogonal projection operator.

Theorem 2.1 *If $u \in H_A^s(\Omega)$, then for any $0 \le \mu \le s$,*

$$\|u-P_N u\|_{H_A^\mu(\Omega)} \le cN^{\frac{\mu-s}{2}}\|u\|_{H_A^s(\Omega)}.$$

Proof For any integers μ and s with $0 \le \mu \le s$,

$$\begin{aligned}\|u-P_N u\|^2_{H_A^\mu(\Omega)}&=\sum_{m,l=N+1}^{\infty}\big(\mu_m^r+\mu_l^z\big)^\mu|u_{ml}|^2+\sum_{m=0}^{N}\sum_{l=N+1}^{\infty}\big(\mu_m^r+\mu_l^z\big)^\mu|u_{ml}|^2\\&\quad+\sum_{m=N+1}^{\infty}\sum_{l=0}^{N}\big(\mu_m^r+\mu_l^z\big)^\mu|u_{ml}|^2\\&\le cN^{\mu-s}\sum_{m,l=0}^{\infty}\big(\mu_m^r+\mu_l^z\big)^s|u_{ml}|^2=cN^{\mu-s}\|u\|^2_{H_A^s(\Omega)}.\end{aligned}\tag{2.33}$$

This with a standard space interpolation technique leads to the desired result. □

We are now in position to study the interpolation operator. The scaled Laguerre–Hermite–Gauss interpolant $\mathcal{I}_N : C(\Omega) \to X_N$ is determined by

$$\mathcal{I}_N u(r_j,z_k)=u(r_j,z_k),\quad 0\le j,k\le N.$$

Clearly, $\mathcal{I}_N u = \mathcal{I}_N^r\mathcal{I}_N^z u$. Hence by (2.6), (2.11), and the equivalence of the norms, a direct calculation shows that

$$\begin{aligned}\|\mathcal{I}_N u\|^2_{L^2(\Omega)}&\le cN^{-1}\Big(\int_\Omega|\partial_r u|^2r^{-1}\,\mathrm{d}r\,\mathrm{d}z+N^{-\frac13}\int_\Omega|\partial_z\partial_r u|^2r^{-1}\,\mathrm{d}r\,\mathrm{d}z\Big)\\&\quad+c\ln N\Big(\int_\Omega|u|^2\big(r+r^3\big)\,\mathrm{d}r\,\mathrm{d}z+N^{-\frac13}\int_\Omega|\partial_z u|^2\big(r+r^3\big)\,\mathrm{d}r\,\mathrm{d}z\\&\quad+\int_\Omega|\partial_r u|^2r\,\mathrm{d}r\,\mathrm{d}z+N^{-\frac13}\int_\Omega|\partial_z\partial_r u|^2r\,\mathrm{d}r\,\mathrm{d}z\Big)\\&\le cN^{-1}\big(\|u\|^2_{H_C^1(\mathbb{R}^3)}+N^{-\frac13}\|u\|^2_{H_C^2(\mathbb{R}^3)}\big)\\&\quad+c\ln N\big(\|u\|^2_{H_C^1(\mathbb{R}^3)}+N^{-\frac13}\|u\|^2_{H_C^2(\mathbb{R}^3)}\big)\end{aligned}$$

$$\leq c \ln N\left(\|u\|^2_{H^1_A(\Omega)} + N^{-\frac{1}{3}}\|u\|^2_{H^2_A(\Omega)}\right). \tag{2.34}$$

Theorem 2.2 *If $u \in H^s_A(\Omega)$, then for any $0 \leq \mu \leq s$ and $s \geq 2$,*

$$\|u - \mathcal{I}_N u\|_{H^\mu_A(\Omega)} \leq c(\ln N)^{\frac{1}{2}} N^{\frac{5}{6}+\frac{\mu-s}{2}} \|u\|_{H^s_A(\Omega)}.$$

Proof From Theorem 2.1 and Lemma 2.4, for any $0 \leq \mu \leq s$,

$$\begin{aligned}\|u - \mathcal{I}_N u\|_{H^\mu_A(\Omega)} &\leq \|u - P_N u\|_{H^\mu_A(\Omega)} + \left\|\mathcal{I}_N(u - P_N u)\right\|_{H^\mu_A(\Omega)} \\ &\leq cN^{\frac{\mu-s}{2}}\|u\|_{H^s_A(\Omega)} + cN^{\frac{\mu}{2}}\left\|\mathcal{I}_N(u - P_N u)\right\|_{L^2(\Omega)}.\end{aligned}$$

Moreover, by (2.34) and Theorem 2.1, for any $s \geq 2$,

$$\begin{aligned}\left\|\mathcal{I}_N(u - P_N u)\right\|_{L^2(\Omega)} &\leq c(\ln N)^{\frac{1}{2}}\left(N^{\frac{1-s}{2}}\|u\|_{H^s_A(\Omega)} + N^{\frac{5}{6}-\frac{s}{2}}\|u\|_{H^s_A(\Omega)}\right) \\ &\leq c(\ln N)^{\frac{1}{2}} N^{\frac{5}{6}-\frac{s}{2}}\|u\|_{H^s_A(\Omega)}.\end{aligned}$$

Therefore,

$$\|u - \mathcal{I}_N u\|_{H^\mu_A(\Omega)} \leq c(\ln N)^{\frac{1}{2}} N^{\frac{5}{6}+\frac{\mu-s}{2}} \|u\|_{H^s_A(\Omega)}.$$ □

3 A Time-Splitting Laguerre–Hermite Collocation Method

We now describe the time-splitting spectral method in [1] for the three-dimensional (3D) Gross–Pitaevskii equation (GPE) with cylindrical symmetry (1.4). For simplicity, we shall only consider the second-order Strang splitting scheme. It is expected that the technique presented in this paper will eventually enable us to prove error estimates for the fourth-order splitting scheme used in [1].

3.1 Strang Splitting in Time

For the semidiscretization in time, we split the 3D GPE with cylindrical symmetry (1.4) into its linear and nonlinear parts:

$$\mathrm{i}\partial_t \psi(r,z,t) = (\mathcal{A}_r + \mathcal{B}_z)\psi = -\frac{1}{2}\left[\frac{1}{r}\partial_r(r\partial_r\psi) + \partial_z^2\psi\right] + \frac{1}{2}\left(\gamma_r^2 r^2 + \gamma_z^2 z^2\right)\psi, \tag{3.1}$$

$$\mathrm{i}\partial_t \psi(r,z,t) = \beta\left|\psi(r,z,t)\right|^2\psi(r,z,t). \tag{3.2}$$

Equations (3.1) and (3.2) are exactly solvable since $|\psi|$ is invariant in time along the solution of (3.2). For a given time step $\tau > 0$, let $t_n = n\tau$, $n = 0, 1, \ldots$, and let ψ^n be the approximation of $\psi(t_n)$. Then, the second-order Strang splitting in time for (1.4) is as follows:

$$\psi^{n+1} = \Phi^\tau\left(\psi^n\right) := \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\mathrm{e}^{-\mathrm{i}\tau\beta|\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\psi^n|^2}\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\psi^n, \tag{3.3}$$

where $\psi^0 = \psi_0$.

3.2 Full Discretization

Before we present the full discretization of (1.4), let us describe the semidiscretization in space using the Laguerre–Hermite collocation method. Find $\psi_N(r,z,t) \in X_N$, i.e.,

$$\psi_N(r,z,t) = \sum_{m,l=0}^{N} \psi_{ml}(t) l_m(r) h_l(z), \tag{3.4}$$

such that

$$\begin{aligned} &\mathrm{i}\partial_t \psi_N(r_j,z_k,t) = (\mathcal{A}_r + \mathcal{B}_z)\psi_N(r_j,z_k,t) + \beta\big|\psi_N(r_j,z_k,t)\big|^2 \psi_N(r_j,z_k,t), \\ &\quad \forall 0 \le j,k \le N, \end{aligned} \tag{3.5}$$

where $\psi_N(r_j,z_k,0) = \psi_0(r_j,z_k)$.

The system (3.5) can also be rewritten as

$$\begin{cases} \mathrm{i}\partial_t \psi_N(r,z,t) = (\mathcal{A}_r + \mathcal{B}_z)\psi_N(r,z,t) + \beta \mathcal{I}_N(|\psi_N(r,z,t)|^2 \psi_N(r,z,t)), \\ \psi_N(r,z,0) = \mathcal{I}_N \psi_0(r,z). \end{cases} \tag{3.6}$$

We now combine the semidiscretization in time in Sect. 3.1 with the semidiscretization in space to obtain a full discretization of (1.4). To do this, we split the space-discretized equation (3.6) into its linear and nonlinear parts:

$$\mathrm{i}\partial_t \psi_N(r,z,t) = (\mathcal{A}_r + \mathcal{B}_z)\psi_N(r,z,t), \tag{3.7}$$

$$\mathrm{i}\partial_t \psi_N(r,z,t) = \beta \mathcal{I}_N\big(\big|\psi_N(r,z,t)\big|^2 \psi_N(r,z,t)\big). \tag{3.8}$$

Clearly, $|\psi_N(r_j,z_k,t)|$ is conserved in time. Thus, the fully discrete Laguerre–Hermite Strang time-splitting scheme is as follows:

$$\begin{aligned} &\psi_N^0(r,z) = \mathcal{I}_N \psi_0(r,z); \\ &\psi_N^{n+1} = \Phi_N^\tau\big(\psi_N^n\big) := \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)} \mathcal{I}_N\big(\mathrm{e}^{-\mathrm{i}\tau\beta|\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\psi_N^n|^2} \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\psi_N^n\big), \\ &\quad n \ge 0. \end{aligned} \tag{3.9}$$

Define the discrete inner product

$$\langle u,v\rangle_N = \sum_{j,k=0}^{N} \omega_j^r \omega_k^z u(r_j,z_k)\overline{v}(r_j,z_k).$$

According to (2.4), (2.5), (2.9), and (2.10), we have

$$\langle \phi,\psi\rangle_N = (\phi,\psi)_\Omega, \quad \forall \phi\psi \in X_{2N+1}. \tag{3.10}$$

Then, we can rewrite (3.9) in a more computationally friendly algorithm: Given $\{\psi_N^n(r_j, x_k)\}$, compute

$$\begin{aligned}
\psi_N^{(1)}(r_j, z_k) &= \sum_{m,l=0}^{N} \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mu_m^r+\mu_l^z)} \widehat{U}_{ml} l_m(r_j) h_l(z_k), \\
\psi_N^{(2)}(r_j, z_k) &= \mathrm{e}^{-\mathrm{i}\tau\beta|\psi_N^{(1)}(r_j,z_k)|^2} \psi_N^{(1)}(r_j, z_k), \\
\psi_N^{n+1}(r_j, z_k) &= \sum_{m,l=0}^{N} \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mu_m^r+\mu_l^z)} \widehat{V}_{ml} l_m(r_j) h_l(z_k),
\end{aligned} \tag{3.11}$$

where

$$\widehat{U}_{ml} = \langle \psi_N^n, l_m h_l \rangle_N = \sum_{j,k=0}^{N} \omega_j^r \omega_k^z \psi_N^n(r_j, z_k) l_m(r_j) h_l(z_k),$$

$$\widehat{V}_{ml} = \langle \psi_N^{(2)}, l_m h_l \rangle_N = \sum_{j,k=0}^{N} \omega_j^r \omega_k^z \psi_N^{(2)}(r_j, z_k) l_m(r_j) h_l(z_k).$$

4 Error Analysis for the Semidiscrete Strang Splitting Scheme

In this section, we shall derive error bounds for the semidiscretization scheme (3.3). We follow the basic procedure in [18], and generalize the error estimates to the $H_A^k(\Omega)$-norms.

We start by establishing a lemma which is needed for dealing with nonlinear terms.

Lemma 4.1 *The following inequalities hold*:

$$\|uvw\|_{L^2(\Omega)} \le c\|u\|_{H_A^1(\Omega)}\|v\|_{H_A^1(\Omega)}\|w\|_{H_A^1(\Omega)}, \tag{4.1}$$

$$\|uvw\|_{L^2(\Omega)} \le c\|u\|_{L^2(\Omega)}\|v\|_{H_A^2(\Omega)}\|w\|_{H_A^2(\Omega)}, \tag{4.2}$$

$$\|uvw\|_{H_A^1(\Omega)} \le c\|u\|_{H_A^1(\Omega)}\|v\|_{H_A^2(\Omega)}\|w\|_{H_A^2(\Omega)}, \tag{4.3}$$

$$\|uvw\|_{H_A^k(\Omega)} \le c\|u\|_{H_A^k(\Omega)}\|v\|_{H_A^k(\Omega)}\|w\|_{H_A^k(\Omega)}, \quad \forall \text{ integer } k \ge 2. \tag{4.4}$$

Proof For any function $\widetilde{u}(x, y, z)$ in $\mathbb{R}^3$ with cylindrical symmetry, we denote $u(r, z) := \widetilde{u}(x, y, z)$, $(r, z) \in \Omega$. Clearly, in this case, $\gamma_x = \gamma_y = \gamma_r$. Thereby,

$$(\mathcal{B}_x + \mathcal{B}_y)\widetilde{u}(x, y, z) = \frac{1}{2}\big(-\partial_x^2 - \partial_y^2 + \gamma_x^2 x^2 + \gamma_y^2 y^2\big)\widetilde{u}(x, y, z) = \mathcal{A}_r u(r, z),$$

and

$$a(\widetilde{u}, \widetilde{u}) = b(u, u).$$

Accordingly, we have

$$\|\widetilde{u}\|_{H^s_B(\mathbb{R}^3)} = \|u\|_{H^s_B(\Omega)},$$

which implies

$$\|\widetilde{u}\|_{H^s_A(\mathbb{R}^3)} = \|u\|_{H^s_A(\Omega)}.$$

We can then obtain the desired results from the above and Lemma 2.3. □

Lemma 4.2 (Stability) *If* $\psi, \varphi \in H^2_A(\Omega) \cap H^k_A(\Omega)$ *with integer* $k \geq 0$, *then*

$$\left\|\Phi^\tau(\psi) - \Phi^\tau(\varphi)\right\|_{H^k_A(\Omega)} \leq \mathrm{e}^{c\tau(\|\psi\|^2_{H^j_A(\Omega)} + \|\varphi\|^2_{H^j_A(\Omega)})} \|\psi - \varphi\|_{H^k_A(\Omega)},$$

where $j = \max(k, 2)$.

Proof We first consider the cases with $0 \leq k \leq 2$. It is clear that the operator $\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r + \mathcal{B}_z)}$ preserves the norm $\|\cdot\|_{H^s_A(\Omega)}$ for any integer $s \geq 0$, since

$$\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r + \mathcal{B}_z)} l_m(r) h_l(z) = \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mu^r_m + \mu^z_l)} l_m(r) h_l(z).$$

Thereby, we only need to compare $\mathrm{e}^{-\mathrm{i}\tau\beta|\psi|^2}\psi$ and $\mathrm{e}^{-\mathrm{i}\tau\beta|\varphi|^2}\varphi$, which are the solutions at time τ of the linear initial value problems:

$$\mathrm{i}\partial_t\theta = \beta|\psi|^2\theta, \qquad \theta(0) = \psi, \tag{4.5}$$

$$\mathrm{i}\partial_t\eta = \beta|\varphi|^2\eta, \qquad \eta(0) = \varphi. \tag{4.6}$$

We first establish a bound for $\|\theta(t)\|_{H^2_A(\Omega)}$. By (4.5) we have

$$\mathrm{i}\big((\mathcal{A}_r + \mathcal{B}_z)\partial_t\theta, (\mathcal{A}_r + \mathcal{B}_z)\theta\big)_\Omega = \beta\big((\mathcal{A}_r + \mathcal{B}_z)\big(|\psi|^2\theta\big), (\mathcal{A}_r + \mathcal{B}_z)\theta\big)_\Omega.$$

Taking the imaginary part in the above, we obtain

$$\partial_t\left\|\theta(t)\right\|^2_{H^2_A(\Omega)} \leq 2\beta\left\||\psi|^2\theta(t)\right\|_{H^2_A(\Omega)}\left\|\theta(t)\right\|_{H^2_A(\Omega)},$$

which implies that

$$\partial_t\left\|\theta(t)\right\|_{H^2_A(\Omega)} \leq \beta\left\||\psi|^2\theta(t)\right\|_{H^2_A(\Omega)}.$$

On the other hand, by (4.4) we obtain

$$\left\||\psi|^2\theta(t)\right\|_{H^2_A(\Omega)} \leq c\|\psi\|^2_{H^2_A(\Omega)}\left\|\theta(t)\right\|_{H^2_A(\Omega)}.$$

A combination of the previous two inequalities leads to

$$\left\|\theta(t)\right\|_{H^2_A(\Omega)} \leq \|\psi\|_{H^2_A(\Omega)} + c\int_0^t \|\psi\|^2_{H^2_A(\Omega)}\left\|\theta(\xi)\right\|_{H^2_A(\Omega)}\mathrm{d}\xi.$$

Applying the usual Gronwall inequality, we obtain

$$\big\|\theta(t)\big\|_{H_A^2(\Omega)} \le \mathrm{e}^{ct\|\psi\|^2_{H_A^2(\Omega)}} \|\psi\|_{H_A^2(\Omega)}. \tag{4.7}$$

Next, by (4.5) and (4.6), we have

$$\mathrm{i}\partial_t(\theta-\eta) = \beta(\psi-\varphi)\overline{\psi}\theta + \beta\varphi(\overline{\psi}-\overline{\varphi})\theta + \beta|\varphi|^2(\theta-\eta). \tag{4.8}$$

We now proceed to treat different cases separately.

(i) $k=0$. By taking the inner product in (4.8) with $\theta-\eta$, and then taking the imaginary part, we get

$$\partial_t\|\theta-\eta\|_{L^2(\Omega)} \le \beta\big\|(\psi-\varphi)\overline{\psi}\theta + \varphi(\overline{\psi}-\overline{\varphi})\theta\big\|_{L^2(\Omega)}.$$

The above with (4.2) yields

$$\partial_t\|\theta-\eta\|_{L^2(\Omega)} \le c\|\psi-\varphi\|_{L^2(\Omega)}\|\theta\|_{H_A^2(\Omega)}\big(\|\psi\|_{H_A^2(\Omega)} + \|\varphi\|_{H_A^2(\Omega)}\big).$$

Integrating the above from 0 to τ and using (4.7), we obtain

$$\begin{aligned}\big\|\theta(\tau)-\eta(\tau)\big\|_{L^2(\Omega)} &\le \|\psi-\varphi\|_{L^2(\Omega)} \\ &\quad + c\tau\|\psi-\varphi\|_{L^2(\Omega)}\big(\|\psi\|^2_{H_A^2(\Omega)} + \|\varphi\|^2_{H_A^2(\Omega)}\big)\mathrm{e}^{c\tau\|\psi\|^2_{H_A^2(\Omega)}} \\ &\le \big(1 + c\tau\big(\|\psi\|^2_{H_A^2(\Omega)} + \|\varphi\|^2_{H_A^2(\Omega)}\big)\big)\|\psi-\varphi\|_{L^2(\Omega)}\mathrm{e}^{c\tau\|\psi\|^2_{H_A^2(\Omega)}} \\ &\le \mathrm{e}^{c\tau(\|\psi\|^2_{H_A^2(\Omega)} + \|\varphi\|^2_{H_A^2(\Omega)})}\|\psi-\varphi\|_{L^2(\Omega)}.\end{aligned}$$

(ii) $k=1,2$. By (4.8) we have

$$\begin{aligned}\mathrm{i}(\mathcal{A}_r+\mathcal{B}_z)^{\frac{k}{2}}\partial_t(\theta-\eta) &= \beta(\mathcal{A}_r+\mathcal{B}_z)^{\frac{k}{2}}\big((\psi-\varphi)\overline{\psi}\theta\big) + \beta(\mathcal{A}_r+\mathcal{B}_z)^{\frac{k}{2}}\big(\varphi(\overline{\psi}-\overline{\varphi})\theta\big) \\ &\quad + \beta(\mathcal{A}_r+\mathcal{B}_z)^{\frac{k}{2}}\big(|\varphi|^2(\theta-\eta)\big).\end{aligned} \tag{4.9}$$

Take the inner product in (4.9) with $(\mathcal{A}_r+\mathcal{B}_z)^{\frac{k}{2}}(\theta-\eta)$. From (4.3) and (4.4), and using an argument similar to the case $k=0$, we get

$$\begin{aligned}\partial_t\|\theta-\eta\|_{H_A^k(\Omega)} &\le c\|\psi-\varphi\|_{H_A^k(\Omega)}\|\theta\|_{H_A^2(\Omega)}\big(\|\psi\|_{H_A^2(\Omega)} + \|\varphi\|_{H_A^2(\Omega)}\big) \\ &\quad + c\|\varphi\|^2_{H_A^2(\Omega)}\|\theta-\eta\|_{H_A^k(\Omega)}.\end{aligned}$$

Therefore, by (4.7) and the Gronwall inequality, we obtain the desired result.

(iii) $k>2$. By a similar argument as before, we can establish the bound on $\|\theta(t)\|_{H_A^k(\Omega)}$, namely,

$$\big\|\theta(t)\big\|_{H_A^k(\Omega)} \le \mathrm{e}^{ct\|\psi\|^2_{H_A^k(\Omega)}}\|\psi\|_{H_A^k(\Omega)}, \quad k\ge 2. \tag{4.10}$$

Thus by (4.10), (4.4), and the Gronwall inequality, we obtain the result with integer $k > 2$. □

We are now in position to estimate the local error. To this end, we denote

$$\widehat{T}(\psi) = -\mathrm{i}(\mathcal{A}_r + \mathcal{B}_z)\psi, \qquad \widehat{V}(\psi) = -\mathrm{i}\beta|\psi|^2\psi. \tag{4.11}$$

Their Lie commutator (cf. [12, 15]) is as follows:

$$\begin{aligned}[\widehat{T}, \widehat{V}](\psi) &= \widehat{T}'(\psi)\widehat{V}(\psi) - \widehat{V}'(\psi)\widehat{T}(\psi) \\ &= -\beta(\mathcal{A}_r + \mathcal{B}_z)\big(|\psi|^2\psi\big) - \beta\psi^2(\mathcal{A}_r + \mathcal{B}_z)\overline{\psi} \\ &\quad + 2\beta|\psi|^2(\mathcal{A}_r + \mathcal{B}_z)\psi. \end{aligned} \tag{4.12}$$

Lemma 4.3 *For any $\psi \in H_A^{k+2}(\Omega)$ with integer $k \geq 0$, we have*

$$\big\|[\widehat{T}, \widehat{V}](\psi)\big\|_{H_A^k(\Omega)} \leq c\|\psi\|^3_{H_A^{k+2}(\Omega)}. \tag{4.13}$$

If, in addition, $\psi \in H_A^{k+4}(\Omega)$, then

$$\big\|\big[\widehat{T}, [\widehat{T}, \widehat{V}]\big](\psi)\big\|_{H_A^k(\Omega)} \leq c\|\psi\|^3_{H_A^{k+4}(\Omega)}. \tag{4.14}$$

Proof Using (4.12) and (4.2)–(4.4), we obtain that

$$\begin{aligned}\big\|[\widehat{T}, \widehat{V}](\psi)\big\|_{H_A^k(\Omega)} &\leq c\big\||\psi|^2\psi\big\|_{H_A^{k+2}(\Omega)} + c\big\|\psi^2(\mathcal{A}_r + \mathcal{B}_z)\overline{\psi}\big\|_{H_A^k(\Omega)} \\ &\quad + c\big\||\psi|^2(\mathcal{A}_r + \mathcal{B}_z)\psi\big\|_{H_A^k(\Omega)} \\ &\leq c\|\psi\|^3_{H_A^{k+2}(\Omega)}. \end{aligned} \tag{4.15}$$

Next, we derive a bound for the following commutator (cf. [12, 15]):

$$\big[\widehat{T}, [\widehat{T}, \widehat{V}]\big](\psi) = \widehat{T}\big([\widehat{T}, \widehat{V}](\psi)\big) - [\widehat{T}, \widehat{V}]'(\psi)\widehat{T}(\psi).$$

By (4.11) and (4.15) we have

$$\big\|\widehat{T}\big([\widehat{T}, \widehat{V}](\psi)\big)\big\|_{H_A^k(\Omega)} = \big\|[\widehat{T}, \widehat{V}](\psi)\big\|_{H_A^{k+2}(\Omega)} \leq c\|\psi\|^3_{H_A^{k+4}(\Omega)}.$$

A direct calculation shows that

$$\begin{aligned}[\widehat{T}, \widehat{V}]'(\psi)\widehat{T}(\psi) &= -\beta(\mathcal{A}_r + \mathcal{B}_z)\big(\psi^2\overline{\widehat{T}(\psi)} + 2|\psi|^2\widehat{T}(\psi)\big) \\ &\quad - \beta\psi^2(\mathcal{A}_r + \mathcal{B}_z)\overline{\widehat{T}(\psi)} + 2\beta\psi\widehat{T}(\psi)(\mathcal{A}_r + \mathcal{B}_z)\overline{\psi} \\ &\quad + 2\beta\big(\psi\overline{\widehat{T}(\psi)}(\mathcal{A}_r + \mathcal{B}_z)\psi + \widehat{T}(\psi)\overline{\psi}(\mathcal{A}_r + \mathcal{B}_z)\psi \\ &\quad + |\psi|^2(\mathcal{A}_r + \mathcal{B}_z)\widehat{T}(\psi)\big). \end{aligned}$$

Furthermore, by (4.4) and (4.11),

$$\left\|(\mathcal{A}_r+\mathcal{B}_z)\big(\psi^2\overline{\widehat{T}(\psi)}\big)\right\|_{H_A^k(\Omega)}=\left\|\psi^2\overline{\widehat{T}(\psi)}\right\|_{H_A^{k+2}(\Omega)}\le c\|\psi\|^2_{H_A^{k+2}(\Omega)}\left\|\overline{\widehat{T}(\psi)}\right\|_{H_A^{k+2}(\Omega)}$$
$$=c\|\psi\|^2_{H_A^{k+2}(\Omega)}\|\psi\|_{H_A^{k+4}(\Omega)}.$$

By using (4.2)–(4.4) and (4.11), the same results can be derived for the estimates of the other terms in $[\widehat{T},\widehat{V}]'(\psi)\widehat{T}(\psi)$. Therefore, we have

$$\left\|[\widehat{T},\widehat{V}]'(\psi)\widehat{T}(\psi)\right\|_{H_A^k(\Omega)}\le c\|\psi\|^2_{H_A^{k+2}(\Omega)}\|\psi\|_{H_A^{k+4}(\Omega)}.$$

A combination of the previous statements leads to the desired result. □

Lemma 4.4 (Local errors) *Let integer* $k\ge 0$*. If the exact solution* $\psi(t)$ *of* (1.4) *is in* $H_A^2(\Omega)\cap H_A^k(\Omega)$ *for all* $0\le t\le\tau$*, and* $\psi_0\in H_A^{k+2}(\Omega)$*, then the local error of the method* (3.3) *is bounded by*

$$\left\|\psi^1-\psi(\tau)\right\|_{H_A^k(\Omega)}\le c\tau^2, \tag{4.16}$$

where c depends only on $\|\psi_0\|_{H_A^{k+2}(\Omega)}$ *and* $\max_{0\le t\le\tau}\|\psi\|_{H_A^j(\Omega)}$ *with* $j=\max(k,2)$*. If, in addition,* $\psi_0\in H_A^{k+4}(\Omega)$*, then*

$$\left\|\psi^1-\psi(\tau)\right\|_{H_A^k(\Omega)}\le c\tau^3, \tag{4.17}$$

where c depends only on $\|\psi_0\|_{H_A^{k+4}(\Omega)}$ *and* $\max_{0\le t\le\tau}\|\psi\|_{H_A^j(\Omega)}$.

The proof of Lemma 4.4 is given in Appendix. The following lemma shall be used for the error analysis.

Lemma 4.5 (Regularity of the numerical solution) *If the exact solution of* (1.4) $\psi(t)\in H_A^{k+2}(\Omega)$ *with integer* $k\ge 2$ *and* $t\in[0,T]$*, then for small enough* τ *and any* $1\le n\le N_0=\frac{T}{\tau}$*, we have*

$$\max_{0\le j\le N_0-n}\left\|\left(\Phi^\tau\right)^n\big(\psi(j\tau)\big)\right\|_{H_A^k(\Omega)}\le T+\max_{0\le t\le T}\left\|\psi(t)\right\|_{H_A^k(\Omega)}.$$

Proof Let

$$E_n=\max_{0\le j\le N_0-n}\left\|\left(\Phi^\tau\right)^n\big(\psi(j\tau)\big)-\left(\Phi^\tau\right)^{n-1}\big(\psi\big((j+1)\tau\big)\big)\right\|_{H_A^k(\Omega)},\quad n\ge 1,$$
$$F_n=\max_{0\le j\le N_0-n}\left\|\left(\Phi^\tau\right)^n\big(\psi(j\tau)\big)\right\|_{H_A^k(\Omega)},\quad n\ge 1,\qquad F_0=\max_{0\le t\le T}\left\|\psi(t)\right\|_{H_A^k(\Omega)}.$$

Then, by (4.16), we deduce that

$$E_1\le c_0\tau^2,$$

where c_0 depends only on $\max_{0\le t\le T}\|\psi(t)\|_{H_A^{k+2}(\Omega)}$. Moreover,

$$\begin{aligned}
F_1 &= \max_{0\le j\le N_0-1}\big\|\Phi^\tau\big(\psi(j\tau)\big)\big\|_{H_A^k(\Omega)}\\
&\le \max_{0\le j\le N_0-1}\big\|\Phi^\tau\big(\psi(j\tau)\big)-\psi\big((j+1)\tau\big)\big\|_{H_A^k(\Omega)}+\max_{0\le j\le N_0-1}\big\|\psi\big((j+1)\tau\big)\big\|_{H_A^k(\Omega)}\\
&\le E_1+F_0.
\end{aligned}$$

Next, due to Lemma 4.2, we have that for $k\ge 2$,

$$E_2=\max_{0\le j\le N_0-2}\big\|\big(\Phi^\tau\big)^2\big(\psi(j\tau)\big)-\Phi^\tau\big(\psi\big((j+1)\tau\big)\big)\big\|_{H_A^k(\Omega)}\le E_1 \mathrm{e}^{c\tau(F_0^2+F_1^2)},$$

and

$$\begin{aligned}
F_2 &= \max_{0\le j\le N_0-2}\big\|\big(\Phi^\tau\big)^2\big(\psi(j\tau)\big)\big\|_{H_A^k(\Omega)}\\
&\le E_2+\max_{0\le j\le N_0-2}\big\|\Phi^\tau\big(\psi\big((j+1)\tau\big)\big)\big\|_{H_A^k(\Omega)}\\
&\le E_2+F_1.
\end{aligned}$$

Finally by induction, we deduce that for $k\ge 2$,

$$\begin{cases} E_n\le E_{n-1}\mathrm{e}^{c\tau(F_{n-1}^2+F_{n-2}^2)}, & n\ge 2,\\ F_n\le E_n+F_{n-1}, & n\ge 1.\end{cases}$$

Thereby,

$$\begin{aligned}
F_n &\le F_{n-1}+E_{n-1}\mathrm{e}^{c\tau(F_{n-1}^2+F_{n-2}^2)}\le\cdots\\
&\le F_{n-1}+E_1\mathrm{e}^{c\tau(F_{n-1}^2+2F_{n-2}^2+\cdots+2F_1^2+F_0^2)}\\
&= F_{n-1}+c_0\tau^2\mathrm{e}^{c\tau(F_{n-1}^2+2F_{n-2}^2+\cdots+2F_1^2+F_0^2)},\quad n\ge 1.
\end{aligned}$$

Now let τ be small enough such that

$$c_0\tau\mathrm{e}^{4cTF_0^2+4cT^3}\le 1. \tag{4.18}$$

Then by induction, we derive that

$$F_n\le F_{n-1}+\tau.$$

Therefore,

$$F_n\le F_0+n\tau\le F_0+T,\quad 1\le n\le N_0.$$

Thus we obtain the desired result. □

Remark 4.1 The condition (4.18) for τ is sufficient but not necessary.

We now present the main result for the Strang splitting scheme (3.3).

Theorem 4.1 *Suppose that integer $k \geq 0$, τ is small enough, and the exact solution $\psi(t)$ of (1.4) is in $H_A^4(\Omega) \cap H_A^{k+2}(\Omega)$ for all $0 \leq t \leq T$. Then the numerical solution ψ^n given by the splitting scheme (3.3) with step size $\tau > 0$ has the following error bound*:

$$\left\| \psi^n - \psi(t_n) \right\|_{H_A^k(\Omega)} \leq c\tau, \quad t_n = n\tau \leq T,$$

where c depends only on T and $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^{k+2}(\Omega)}$. If, in addition, $\psi(t) \in H_A^{k+4}(\Omega)$ for all $0 \leq t \leq T$, then

$$\left\| \psi^n - \psi(t_n) \right\|_{H_A^k(\Omega)} \leq c\tau^2, \quad t_n = n\tau \leq T,$$

where c depends only on T and $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^{k+4}(\Omega)}$.

Proof According to Lemma 4.5, if $\psi \in H_A^4(\Omega) \cap H_A^{k+2}(\Omega)$ with $k \geq 0$, then for $m = \max(k, 2)$,

$$\max_{0 \leq j \leq N_0 - n} \left\| \left(\Phi^\tau\right)^n \left(\psi(j\tau)\right) \right\|_{H_A^m(\Omega)} \leq T + \max_{0 \leq t \leq T} \|\psi\|_{H_A^m(\Omega)}.$$

Therefore, by Lemma 4.2, (4.16), and the previous inequality, and using the standard argument of Lady Windermere's fan (cf. [12]), we obtain that

$$\begin{aligned}
\left\| \psi^n - \psi(n\tau) \right\|_{H_A^k(\Omega)} &\leq \sum_{j=0}^{n-1} \Big\| \left(\Phi^\tau\right)^{n-j-1} \left(\Phi^\tau\left(\psi(j\tau)\right)\right) \\
&\quad - \left(\Phi^\tau\right)^{n-j-1} \left(\psi\left((j+1)\tau\right)\right) \Big\|_{H_A^k(\Omega)} \\
&\leq n e^{c_1 T} \max_{0 \leq j \leq n-1} \left\| \Phi^\tau\left(\psi(j\tau)\right) - \psi\left((j+1)\tau\right) \right\|_{H_A^k(\Omega)} \\
&\leq c_2 T e^{c_1 T} \tau,
\end{aligned}$$

where c_1 depends only on T and $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^m(\Omega)}$, and c_2 depends only on $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^{k+2}(\Omega)}$. If, in addition, $\psi(t) \in H_A^{k+4}(\Omega)$ for all $0 \leq t \leq T$, then we obtain from (4.17) that

$$\left\| \psi^n - \psi(n\tau) \right\|_{H_A^k(\Omega)} \leq c_3 T e^{c_1 T} \tau^2,$$

where c_3 depends only on $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^{k+4}(\Omega)}$. This completes the proof. □

5 Error Analysis of the Fully Discrete Strang Splitting Laguerre–Hermite Collocation Scheme

In this section, we present error bounds for the full-discretization scheme (3.9).

Lemma 5.1 *We are given* $\psi \in X_N$. *Then for* $\varphi \in H_A^s(\Omega)$ *with integer* $s \geq 2$,

$$\begin{aligned}&\big\|\Phi_N^\tau(\psi) - P_N\Phi^\tau(\varphi)\big\|_{L^2(\Omega)}^2\\&\quad\leq \exp\big(c\tau\|\psi\|_{H_A^2(\Omega)}\|\varphi\|_{H_A^2(\Omega)}\exp\big(c\tau\|\varphi\|_{H_A^2(\Omega)}^2\big)\big)\|\psi - P_N\varphi\|_{L^2(\Omega)}^2\\&\qquad + c\tau^2 N^{\frac{3}{2}-s}\|\varphi\|_{H_A^2(\Omega)}^2\|\varphi\|_{H_A^s(\Omega)}^4\\&\qquad \times \exp\big(c\tau\|\varphi\|_{H_A^s(\Omega)}^2 + c\tau\|\psi\|_{H_A^2(\Omega)}\|\varphi\|_{H_A^2(\Omega)}\exp\big(c\tau\|\varphi\|_{H_A^2(\Omega)}^2\big)\big).\end{aligned}$$

Proof We consider the errors in its linear and nonlinear parts, respectively. We first consider the errors of the linear parts:

$$\mathrm{i}\partial_t\theta = (\mathcal{A}_r + \mathcal{B}_z)\theta, \qquad \theta(0) = \psi, \tag{5.1}$$

$$\mathrm{i}\partial_t\eta = (\mathcal{A}_r + \mathcal{B}_z)\eta, \qquad \eta(0) = \varphi, \tag{5.2}$$

where θ and η correspond to the solutions of the linear parts of the full discretization and the semidiscretization in time, respectively. From (5.2) and (2.32) we further obtain

$$\begin{aligned}&\mathrm{i}(\partial_t P_N\eta, \phi)_\Omega = \mathrm{i}(\partial_t\eta, \phi)_\Omega = \big((\mathcal{A}_r + \mathcal{B}_z)\eta, \phi\big)_\Omega = \big((\mathcal{A}_r + \mathcal{B}_z)P_N\eta, \phi\big)_\Omega,\\&\quad\forall\phi \in X_N.\end{aligned}$$

Therefore,

$$\mathrm{i}\big(\partial_t(\theta - P_N\eta), \phi\big)_\Omega = \big((\mathcal{A}_r + \mathcal{B}_z)(\theta - P_N\eta), \phi\big)_\Omega, \quad \forall\phi \in X_N. \tag{5.3}$$

Taking $\phi = (\mathcal{A}_r + \mathcal{B}_z)^k(\theta - P_N\eta)$ ($\in X_N$) in the above, we obtain from its imaginary part that

$$\partial_t\|\theta - P_N\eta\|_{H_A^k(\Omega)}^2 = 0,$$

whence

$$\big\|\theta(\cdot,t) - (P_N\eta)(\cdot,t)\big\|_{H_A^k(\Omega)} = \|\psi - P_N\varphi\|_{H_A^k(\Omega)}, \quad 0 \leq t \leq \tau. \tag{5.4}$$

Next let $\tilde{\psi} \in X_N$ and consider the errors of the nonlinear parts:

$$\mathrm{i}\partial_t\theta = \beta\mathcal{I}_N\big(|\theta|^2\theta\big), \qquad \theta(0) = \tilde{\psi}, \tag{5.5}$$

$$\mathrm{i}\partial_t\eta = \beta|\eta|^2\eta, \qquad \eta(0) = \tilde{\varphi}. \tag{5.6}$$

From (5.5) and (5.6), one verifies readily that $|\theta(r_j, z_k, t)| = |\tilde{\psi}(r_j, z_k)|$, $|\eta(r, z, t)| = |\tilde{\varphi}(r, z)|$ and

$$\mathrm{i}\partial_t(\theta - P_N\eta) = \beta\mathcal{I}_N\big(\big(|\theta|^2 + |P_N\eta|^2\big)(\theta - P_N\eta) + \theta P_N\eta(\overline{\theta} - \overline{P_N\eta})$$

$$+ |P_N\eta|^2 P_N\eta\big) - \beta P_N\big(|\eta|^2\eta\big).$$

Thus

$$\begin{aligned} &\mathrm{i}\big(\partial_t(\theta - P_N\eta), \phi\big)_\Omega \\ &\quad = \beta\big\langle\big(|\theta|^2 + |P_N\eta|^2\big)(\theta - P_N\eta), \phi\big\rangle_N \\ &\qquad + \beta\big\langle\theta P_N\eta(\overline{\theta} - \overline{P_N\eta}), \phi\big\rangle_N \\ &\qquad + \beta\big\langle|P_N\eta|^2 P_N\eta, \phi\big\rangle_N - \beta\big(|\eta|^2\eta, \phi\big)_\Omega, \quad \forall\phi \in X_N. \end{aligned} \tag{5.7}$$

Next let $M = [\frac{N}{3}]$. To deal with the cubic term, we need to consider a special orthogonal projection, similar to (2.31), but with $\frac{\gamma_r}{3}$ and $\frac{\gamma_z}{3}$ in place of γ_r and γ_z. For clarity, we denote it by $\widetilde{P}_M\colon L^2(\Omega) \to X_M(\gamma_r/3, \gamma_z/3)$. More specifically,

$$(u - \widetilde{P}_M u, \phi)_\Omega = 0, \quad \forall\phi \in X_M(\gamma_r/3, \gamma_z/3). \tag{5.8}$$

In particular, we have the following attractive property:

$$\begin{aligned} &|\widetilde{P}_M\tilde{\psi}|^2\widetilde{P}_M\eta \in X_N(\gamma_r, \gamma_z) \quad \text{and} \\ &\big\langle|\widetilde{P}_M\tilde{\psi}|^2\widetilde{P}_M\eta, \theta - P_N\eta\big\rangle_N = \big(|\widetilde{P}_M\tilde{\psi}|^2\widetilde{P}_M\eta, \theta - P_N\eta\big)_\Omega. \end{aligned}$$

Moreover, the same estimate in Theorem 2.1 holds for this variation. Hence, taking $\phi = \theta - P_N\eta$ $(\in X_N)$ in (5.7), we obtain from its imaginary part that

$$\begin{aligned} \partial_t\|\theta - P_N\eta\|^2_{L^2(\Omega)} &\le 2\beta\big|\big\langle\theta P_N\eta(\overline{\theta} - \overline{P_N\eta}), \theta - P_N\eta\big\rangle_N + \big\langle|P_N\eta|^2 P_N\eta, \theta - P_N\eta\big\rangle_N \\ &\qquad - \big(|\eta|^2\eta, \theta - P_N\eta\big)_\Omega\big| \\ &\le 2\beta\sum_{j=1}^{3}|G_j|, \end{aligned} \tag{5.9}$$

where

$$\begin{aligned} G_1 &= \big\langle\theta P_N\eta(\overline{\theta} - \overline{P_N\eta}), \theta - P_N\eta\big\rangle_N, \\ G_2 &= \big\langle|P_N\eta|^2 P_N\eta - |\widetilde{P}_M\eta|^2\widetilde{P}_M\eta, \theta - P_N\eta\big\rangle_N, \\ G_3 &= \big(|\widetilde{P}_M\eta|^2\widetilde{P}_M\eta - |\eta|^2\eta, \theta - P_N\eta\big)_\Omega. \end{aligned}$$

We derive from (5.9) that

$$\|\theta - P_N\eta\|\partial_t\|\theta - P_N\eta\| \le \beta\sum_{j=1}^{3}|G_j|. \tag{5.10}$$

We now estimate $|G_j|$, $j = 1, 2, 3$. For any function $u(r, z)$, $(r, z) \in \Omega$, we denote $\widetilde{u}(x, y, z) := u(r, z)$, $(x, y, z) \in \mathbb{R}^3$. Then, by using a Sobolev inequality (cf., for instance, [7]) and the equivalence of norms (cf. Lemma 2.1), we obtain that for any

$u \in H_A^m(\Omega)$ with integer $m > \frac{3}{2}$,

$$\begin{aligned}\|u\|_{L^\infty(\Omega)} = \|\widetilde{u}\|_{L^\infty(\mathbb{R}^3)} &\le c\|\partial_x^m \widetilde{u}\|_{L^2(\mathbb{R}^3)}^{\frac{3}{2m}} \|\widetilde{u}\|_{L^2(\mathbb{R}^3)}^{1-\frac{3}{2m}} \\ &\le c\|\widetilde{u}\|_{H_A^m(\mathbb{R}^3)}^{\frac{3}{2m}} \|\widetilde{u}\|_{L^2(\mathbb{R}^3)}^{1-\frac{3}{2m}} = c\|u\|_{H_A^m(\Omega)}^{\frac{3}{2m}} \|u\|_{L^2(\Omega)}^{1-\frac{3}{2m}}, \end{aligned} \tag{5.11}$$

which implies in particular that

$$\|u\|_{L^\infty(\Omega)} \le C\|u\|_{H_A^2(\Omega)}. \tag{5.12}$$

Due to $|\theta(r_j, z_k, t)| = |\tilde{\psi}(r_j, z_k)|$, we have

$$\begin{aligned}|G_1| &\le \|\tilde{\psi}\|_{L^\infty(\Omega)} \|P_N\eta\|_{L^\infty(\Omega)} \|\theta - P_N\eta\|_{L^2(\Omega)}^2 \\ &\le c\|\tilde{\psi}\|_{H_A^2(\Omega)} \|\eta\|_{H_A^2(\Omega)} \|\theta - P_N\eta\|_{L^2(\Omega)}^2. \end{aligned} \tag{5.13}$$

Moreover,

$$\begin{aligned}|G_2| &= \Big|\Big\langle |P_N\eta|^2(P_N\eta - \widetilde{P}_M\eta) + \overline{P_N\eta}\widetilde{P}_M\eta(P_N\eta - \widetilde{P}_M\eta) \\ &\quad + P_N\eta\widetilde{P}_M\eta(\overline{P_N\eta} - \overline{\widetilde{P}_M\eta}) - \widetilde{P}_M\eta|P_N\eta - \widetilde{P}_M\eta|^2, \theta - P_N\eta\Big\rangle_N\Big| \\ &\le \big(\|P_N\eta\|_{L^\infty(\Omega)} + \|\widetilde{P}_M\eta\|_{L^\infty(\Omega)}\big)\|P_N\eta - \widetilde{P}_M\eta\|_{L^\infty(\Omega)}\|P_N\eta\|_{L^2(\Omega)} \\ &\quad \times \|\theta - P_N\eta\|_{L^2(\Omega)} \\ &\quad + \|P_N\eta - \widetilde{P}_M\eta\|_{L^\infty(\Omega)}^2 \|\mathcal{I}_N\widetilde{P}_M\eta\|_{L^2(\Omega)}\|\theta - P_N\eta\|_{L^2(\Omega)}. \end{aligned}$$

By (5.11) and Theorem 2.1 we obtain that for $s > \frac{3}{2}$,

$$\begin{aligned}&\|P_N\eta - \widetilde{P}_M\eta\|_{L^\infty(\Omega)} \\ &\quad \le c\|P_N\eta - \widetilde{P}_M\eta\|_{H_A^s(\Omega)}^{\frac{3}{2s}} \|P_N\eta - \widetilde{P}_M\eta\|_{L^2(\Omega)}^{1-\frac{3}{2s}} \\ &\quad \le c\big(\|P_N\eta - \eta\|_{H_A^s(\Omega)} + \|\eta - \widetilde{P}_M\eta\|_{H_A^s(\Omega)}\big)^{\frac{3}{2s}} \\ &\qquad \times \big(\|P_N\eta - \eta\|_{L^2(\Omega)} + \|\eta - \widetilde{P}_M\eta\|_{L^2(\Omega)}\big)^{1-\frac{3}{2s}} \\ &\quad \le cN^{\frac{3}{4}-\frac{s}{2}}\|\eta\|_{H_A^s(\Omega)}. \end{aligned} \tag{5.14}$$

Therefore, by the above and (2.34), we can derive

$$|G_2| \le cN^{\frac{3}{4}-\frac{s}{2}}\|\eta\|_{H_A^2(\Omega)}\|\eta\|_{H_A^s(\Omega)}^2\|\theta - P_N\eta\|_{L^2(\Omega)}. \tag{5.15}$$

It is also verified readily that

$$|G_3| \le cN^{-\frac{s}{2}}\|\eta\|_{H_A^2(\Omega)}^2\|\eta\|_{H_A^s(\Omega)}\|\theta - P_N\eta\|_{L^2(\Omega)}. \tag{5.16}$$

Since the operator $\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}$ preserves the norms $\|\cdot\|_{H_A^s(\Omega)}$, we have

$$\|\tilde{\psi}\|_{H_A^s(\Omega)} = \|\psi\|_{H_A^s(\Omega)}, \qquad \|\tilde{\varphi}\|_{H_A^s(\Omega)} = \|\varphi\|_{H_A^s(\Omega)},$$
$$\|\tilde{\psi} - P_N\tilde{\varphi}\|_{L^2(\Omega)} = \|\psi - P_N\varphi\|_{L^2(\Omega)}, \quad \forall s \geq 0.$$

Furthermore, by (4.10), we find

$$\big\|\eta(t)\big\|_{H_A^s(\Omega)} \leq \mathrm{e}^{ct\|\varphi\|^2_{H_A^s(\Omega)}}\|\varphi\|_{H_A^s(\Omega)} \leq \mathrm{e}^{c\tau\|\varphi\|^2_{H_A^s(\Omega)}}\|\varphi\|_{H_A^s(\Omega)},$$
$$0 \leq t \leq \tau, \quad \forall \text{ integer } s \geq 2.$$

Hence, a combination of (5.10), (5.13)–(5.16), and (5.4) yields

$$\partial_t\|\theta - P_N\eta\|_{L^2(\Omega)} \leq c\|\psi\|_{H_A^2(\Omega)}\|\varphi\|_{H_A^2(\Omega)}\mathrm{e}^{c\tau\|\varphi\|^2_{H_A^2(\Omega)}}\|\theta - P_N\eta\|_{L^2(\Omega)}$$
$$+ cN^{\frac{3}{4}-\frac{s}{2}}\|\varphi\|_{H_A^2(\Omega)}\|\varphi\|^2_{H_A^s(\Omega)}\mathrm{e}^{c\tau\|\varphi\|^2_{H_A^s(\Omega)}}.$$

Finally, by using the Gronwall inequality and (5.4), we obtain the desired result. □

Theorem 5.1 *We assume* $\psi(t) \in H_A^{s+2}(\Omega)$ $(0 \leq t \leq T)$ *with integer* $s \geq 4$. *Then for* N *sufficiently large and* τ *sufficiently small* (*cf.* (5.21) *below*), *we have for integer* $s-2 < k \leq s$,

$$\big\|\psi_N^n - \psi(t_n)\big\|_{H_A^k(\Omega)} \leq cN^{\frac{3}{4}+\frac{k-s}{2}} + c\tau, \quad 1 \leq n \leq \frac{T}{\tau}; \tag{5.17}$$

and for integer $0 \leq k \leq s-2$,

$$\big\|\psi_N^n - \psi(t_n)\big\|_{H_A^k(\Omega)} \leq cN^{\frac{3}{4}+\frac{k-s}{2}} + c\tau^2, \quad 1 \leq n \leq \frac{T}{\tau}. \tag{5.18}$$

Proof Due to $\psi(t) \in H_A^{s+2}(\Omega)$ with integer $s \geq 4$, we have from Lemma 4.5 that there exists a constant $M_0 > 0$, such that for all $1 \leq n \leq \frac{T}{\tau}$,

$$\big\|\psi^n\big\|_{H_A^s(\Omega)} \leq \frac{M_0}{2}, \tag{5.19}$$

provided that τ is small enough. Without loss of generality, we also assume that $\|\psi_0\|_{H_A^{s+2}(\Omega)} \leq \frac{M_0}{2}$. Next, according to Theorem 2.2, we have

$$\|\psi_0 - \mathcal{I}_N\psi_0\|_{H_A^2(\Omega)} \leq c(\ln N)^{\frac{1}{2}}N^{\frac{5}{6}-\frac{s}{2}}\|\psi_0\|_{H_A^{s+2}}.$$

Hence, we obtain that for large N,

$$\|\mathcal{I}_N\psi_0\|_{H_A^2(\Omega)} \leq \|\psi_0\|_{H_A^2(\Omega)} + \|\psi_0 - \mathcal{I}_N\psi_0\|_{H_A^2(\Omega)} \leq M_0. \tag{5.20}$$

Now let N be large enough and τ be small enough such that

$$c^2 \ln N N^{-\frac{11}{6}} \mathrm{e}^{\frac{1}{2}cTM_0^2 \mathrm{e}^{\frac{1}{4}c\tau M_0^2}} + \frac{1}{16}c^2\tau T M_0^4 \mathrm{e}^{\frac{1}{2}cTM_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \le 1. \tag{5.21}$$

We proceed by induction on n.

(i) $n=1$. By Lemma 5.1, (5.19), (5.20), and Theorems 2.1 and 2.2, we get that

$$\begin{aligned}
&\|\psi_N^1 - P_N\psi^1\|_{L^2(\Omega)}^2 \\
&\quad\le \mathrm{e}^{c\tau\|\mathcal{I}_N\psi_0\|_{H_A^2(\Omega)}\|\psi_0\|_{H_A^2(\Omega)}\mathrm{e}^{c\tau\|\psi_0\|_{H_A^2(\Omega)}^2}} \|\mathcal{I}_N\psi_0 - P_N\psi_0\|_{L^2(\Omega)}^2 \\
&\qquad + c\tau^2 N^{\frac{3}{2}-s}\|\psi_0\|_{H_A^2(\Omega)}^2\|\psi_0\|_{H_A^s(\Omega)}^4 \\
&\qquad \times \mathrm{e}^{c\tau\|\psi_0\|_{H_A^s(\Omega)}^2 + c\tau\|\mathcal{I}_N\psi_0\|_{H_A^2(\Omega)}\|\psi_0\|_{H_A^2(\Omega)}\mathrm{e}^{c\tau\|\psi_0\|_{H_A^2(\Omega)}^2}} \\
&\quad\le \mathrm{e}^{\frac{1}{2}c\tau M_0^2\mathrm{e}^{\frac{1}{4}c\tau M_0^2}}\|\mathcal{I}_N\psi_0 - P_N\psi_0\|_{L^2(\Omega)}^2 + \frac{1}{64}c\tau^2 N^{\frac{3}{2}-s}M_0^6\mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \\
&\quad\le c\ln N N^{-s-\frac{1}{3}}\|\psi_0\|_{H_A^{s+2}(\Omega)}^2 \mathrm{e}^{\frac{1}{2}c\tau M_0^2\mathrm{e}^{\frac{1}{4}c\tau M_0^2}} + \frac{1}{64}c\tau^2 N^{\frac{3}{2}-s}M_0^6\mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \\
&\quad\le \frac{1}{4}c\ln N N^{-s-\frac{1}{3}}M_0^2\mathrm{e}^{\frac{1}{2}c\tau M_0^2\mathrm{e}^{\frac{1}{4}c\tau M_0^2}} + \frac{1}{64}c\tau^2 N^{\frac{3}{2}-s}M_0^6\mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})}.
\end{aligned}$$

This with Lemma 2.4 and (5.21) gives

$$\begin{aligned}
&\|\psi_N^1 - P_N\psi^1\|_{H_A^k(\Omega)}^2 \\
&\quad\le cN^k\|\psi_N^1 - P_N\psi^1\|_{L^2(\Omega)}^2 \\
&\quad\le \frac{1}{4}c^2\ln N N^{k-s-\frac{1}{3}}M_0^2\mathrm{e}^{\frac{1}{2}c\tau M_0^2\mathrm{e}^{\frac{1}{4}c\tau M_0^2}} + \frac{1}{64}c^2\tau^2 N^{k+\frac{3}{2}-s}M_0^6\mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \\
&\quad\le \frac{M_0^2}{4}N^{k+\frac{3}{2}-s}.
\end{aligned} \tag{5.22}$$

In particular, by (5.19) and (5.22) we get that for integer $s\ge 4$,

$$\begin{aligned}
\|\psi_N^1\|_{H_A^2(\Omega)} &\le \|P_N\psi^1\|_{H_A^2(\Omega)} + \|\psi_N^1 - P_N\psi^1\|_{H_A^2(\Omega)} \\
&\le \|\psi^1\|_{H_A^2(\Omega)} + \|\psi_N^1 - P_N\psi^1\|_{H_A^2(\Omega)} \le M_0.
\end{aligned} \tag{5.23}$$

(ii) Next assume that the results (5.22) and (5.23) with $n=m$ hold, namely,

$$\begin{aligned}
&\|\psi_N^m - P_N\psi^m\|_{H_A^k(\Omega)}^2 \\
&\quad\le cN^k\|\psi_N^m - P_N\psi^m\|_{L^2(\Omega)}^2
\end{aligned}$$

$$
\begin{aligned}
&\leq \frac{1}{4}c^2 \ln N N^{k-s-\frac{1}{3}} M_0^2 \mathrm{e}^{\frac{1}{2}mc\tau M_0^2 \mathrm{e}^{\frac{1}{4}c\tau M_0^2}} \\
&\quad + \frac{1}{64}mc^2\tau^2 N^{k+\frac{3}{2}-s} M_0^6 \mathrm{e}^{\frac{1}{2}mc\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \\
&\leq \frac{M_0^2}{4} N^{k+\frac{3}{2}-s},
\end{aligned}
\tag{5.24}
$$

and

$$
\|\psi_N^m\|_{H_A^2(\Omega)} \leq M_0. \tag{5.25}
$$

We now verify the results with $n = m + 1$. Clearly, by Lemma 5.1, (5.25), and (5.19), we derive that

$$
\begin{aligned}
&\|\psi_N^{m+1} - P_N\psi^{m+1}\|_{L^2(\Omega)}^2 \\
&\quad \leq \mathrm{e}^{c\tau\|\psi_N^m\|_{H_A^2(\Omega)}\|\psi^m\|_{H_A^2(\Omega)}\mathrm{e}^{c\tau\|\psi^m\|_{H_A^2(\Omega)}^2}} \|\psi_N^m - P_N\psi^m\|_{L^2(\Omega)}^2 \\
&\qquad + c\tau^2 N^{\frac{3}{2}-s} \|\psi^m\|_{H_A^2(\Omega)}^2 \|\psi^m\|_{H_A^s(\Omega)}^4 \\
&\qquad \times \mathrm{e}^{c\tau\|\psi^m\|_{H_A^s(\Omega)}^2 + c\tau\|\psi_N^m\|_{H_A^2(\Omega)}\|\psi^m\|_{H_A^2(\Omega)}\mathrm{e}^{c\tau\|\psi^m\|_{H_A^2(\Omega)}^2}} \\
&\quad \leq \mathrm{e}^{\frac{1}{2}c\tau M_0^2 \mathrm{e}^{\frac{1}{4}c\tau M_0^2}} \|\psi_N^m - P_N\psi^m\|_{L^2(\Omega)}^2 + \frac{1}{64}c\tau^2 N^{\frac{3}{2}-s} M_0^6 \mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})}.
\end{aligned}
$$

The above with Lemma 2.4 and (5.24) lead to

$$
\begin{aligned}
&\|\psi_N^{m+1} - P_N\psi^{m+1}\|_{H_A^k(\Omega)}^2 \\
&\quad \leq cN^k \|\psi_N^{m+1} - P_N\psi^{m+1}\|_{L^2(\Omega)}^2 \\
&\quad \leq cN^k \mathrm{e}^{\frac{1}{2}c\tau M_0^2 \mathrm{e}^{\frac{1}{4}c\tau M_0^2}} \|\psi_N^m - P_N\psi^m\|_{L^2(\Omega)}^2 \\
&\qquad + \frac{1}{64}c^2\tau^2 N^{k+\frac{3}{2}-s} M_0^6 \mathrm{e}^{\frac{1}{2}c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})} \\
&\quad \leq \frac{1}{4}c^2 \ln N N^{k-s-\frac{1}{3}} M_0^2 \mathrm{e}^{\frac{1}{2}(m+1)c\tau M_0^2 \mathrm{e}^{\frac{1}{4}c\tau M_0^2}} \\
&\qquad + \frac{1}{64}(m+1)c^2\tau^2 N^{k+\frac{3}{2}-s} M_0^6 \mathrm{e}^{\frac{1}{2}(m+1)c\tau M_0^2(\frac{1}{2}+\mathrm{e}^{\frac{1}{4}c\tau M_0^2})}.
\end{aligned}
\tag{5.26}
$$

Hence by (5.21) and (5.26), for $(m+1)\tau \leq T$,

$$
\|\psi_N^{m+1} - P_N\psi^{m+1}\|_{H_A^k(\Omega)}^2 \leq \frac{M_0^2}{4} N^{k+\frac{3}{2}-s}.
$$

In particular, for integer $s \geq 4$,

$$\|\psi_N^{m+1}\|_{H_A^2(\Omega)} \leq \|P_N\psi^{m+1}\|_{H_A^2(\Omega)} + \|\psi_N^{m+1} - P_N\psi^{m+1}\|_{H_A^2(\Omega)}$$
$$\leq \|\psi^{m+1}\|_{H_A^2(\Omega)} + \|\psi_N^{m+1} - P_N\psi^{m+1}\|_{H_A^2(\Omega)} \leq M_0. \quad (5.27)$$

Therefore, we obtain that for integer $s \geq 4$,

$$\|\psi_N^n - P_N\psi^n\|_{H_A^k(\Omega)}^2 \leq \frac{M_0^2}{4}N^{k+\frac{3}{2}-s}, \quad n \leq \frac{T}{\tau}, \tag{5.28}$$

and

$$\|\psi_N^n\|_{H_A^2(\Omega)} \leq M_0, \quad n \leq \frac{T}{\tau}. \tag{5.29}$$

Since

$$\|\psi_N^n - \psi(t_n)\|_{H_A^k(\Omega)} \leq \|\psi_N^n - P_N\psi^n\|_{H_A^k(\Omega)} + \|\psi^n - P_N\psi^n\|_{H_A^k(\Omega)}$$
$$+ \|\psi^n - \psi(t_n)\|_{H_A^k(\Omega)}, \quad (5.30)$$

we use (5.28), Theorem 2.1, (5.19), and Theorem 4.1 successively to derive the results (5.17) and (5.18). □

The restriction on N in (5.21) can be removed if we set $\psi_N^0(r,z) = P_N\psi_0(r,z)$ instead of $\psi_N^0(r,z) = \mathcal{I}_N\psi_0(r,z)$ in (3.9). More precisely, we have the following result.

Corollary 5.1 *Let $\psi_N^0(r,z) = P_N\psi_0(r,z)$ in (3.9) and $\psi(t) \in H_A^{s+2}(\Omega)$ $(0 \leq t \leq T)$ with integer $s \geq 4$. Then for τ sufficiently small such that*

$$\frac{1}{16}c^2\tau T M_0^4 e^{\frac{1}{2}cTM_0^2(\frac{1}{2}+e^{\frac{1}{4}c\tau M_0^2})} \leq 1, \tag{5.31}$$

we have for $s-2 < k \leq s$,

$$\|\psi_N^n - \psi(t_n)\|_{H_A^k(\Omega)} \leq cN^{\frac{3}{4}+\frac{k-s}{2}} + c\tau, \quad 1 \leq n \leq \frac{T}{\tau}; \tag{5.32}$$

and for $0 \leq k \leq s-2$,

$$\|\psi_N^n - \psi(t_n)\|_{H_A^k(\Omega)} \leq cN^{\frac{3}{4}+\frac{k-s}{2}} + c\tau^2, \quad 1 \leq n \leq \frac{T}{\tau}. \tag{5.33}$$

The proof of the above result is essentially the same as that of Theorem 5.1 without using (5.20) and with (5.31) instead of (5.21).

6 The d-Dimensional Gross–Pitaevskii Equation

In this section, we shall present error bounds of the Strang splitting Hermite collocation method for the d-dimensional GPE:

$$\begin{cases} i\partial_t \psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) + \mathbf{x}^2\psi(\mathbf{x},t) + |\psi(\mathbf{x},t)|^2\psi(\mathbf{x},t), \\ \psi(\mathbf{x},0) = \psi_0(\mathbf{x}), \qquad \lim_{|\mathbf{x}|\to\infty}\psi(\mathbf{x},t) = 0, \quad t \ge 0, \end{cases} \tag{6.1}$$

where $\mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ and $\mathbf{x}^2 = x_1^2 + \cdots + x_d^2$.

6.1 Notation and Some Basic Results

For simplicity, we still denote by $h_l(z)$ the one-dimensional Hermite function as defined in (2.7) with $\gamma_z \equiv 1$. For $l = (l_1, \dots, l_d) \in \mathbb{N}^d$, the d-dimensional Hermite function is defined by

$$h_l(\mathbf{x}) = h_{l_1}(x_1)\cdots h_{l_d}(x_d),$$

which satisfies

$$\mathcal{L}h_l(\mathbf{x}) := \left(-\Delta + \mathbf{x}^2\right)h_l(\mathbf{x}) = \mu_l h_l(\mathbf{x}), \quad \mu_l = 2(l_1 + \cdots + l_d) + d.$$

We denote the spaces $L^2(\mathbb{R}^d)$ and $H^s(\mathbb{R}^d)$, $s > 0$ with the inner products, seminorms, and norms as usual. For any $u \in L^2(\mathbb{R}^d)$, we write

$$u(\mathbf{x}) = \sum_{l=0}^{\infty} u_l h_l(\mathbf{x}).$$

As before, the linear differential operator $\mathcal{L}$ is positive definite and self-adjoint. Thus for any u and v in the domain of $\mathcal{L}$,

$$\begin{aligned} (\mathcal{L}u, v)_{\mathbb{R}^d} &= (u, \mathcal{L}v)_{\mathbb{R}^d} = a_d(u,v), \\ (\mathcal{L}u, u)_{\mathbb{R}^d} &= a_d(u,u) > 0, \quad \text{if } u \neq 0, \end{aligned} \tag{6.2}$$

where the bilinear form

$$a_d(u,v) = (\nabla u, \nabla v)_{\mathbb{R}^d} + \left(\mathbf{x}^2 u, v\right)_{\mathbb{R}^d}.$$

In particular,

$$a_d(h_l, h_{l'}) = (\mathcal{L}h_l, h_{l'})_{\mathbb{R}^d} = \mu_l \delta_{ll'}. \tag{6.3}$$

The fractional power $\mathcal{L}^{1/2}$ is well defined, and the associated norms can be characterized by

$$\left\|\mathcal{L}^{1/2}u\right\|_{\mathbb{R}^d}^2 = a_d(u,u), \tag{6.4}$$

$$\left\|\mathcal{L}^{m+1/2}u\right\|_{\mathbb{R}^d}^2 = a_d\left(\mathcal{L}^m u, \mathcal{L}^m u\right), \quad \forall m \in \mathbb{N}. \tag{6.5}$$

We also introduce the following three Sobolev spaces equipped with the norms:

$$\|u\|_{H^s_A(\mathbb{R}^d)} = \left(\sum_{l=0}^{\infty} \mu_l^s |u_l|^2\right)^{\frac{1}{2}}, \qquad \|u\|_{H^s_B(\mathbb{R}^d)} = \left\|\mathcal{L}^{\frac{s}{2}} u\right\|_{L^2(\mathbb{R}^d)},$$

$$\|u\|_{H^s_C(\mathbb{R}^d)} = \left(\sum_{l_1+\cdots+l_d=0}^{s} \left\|\left(x_1^2+\cdots+x_d^2+1\right)^{\frac{s-l_1-\cdots-l_d}{2}} \partial_{x_1}^{l_1}\cdots\partial_{x_d}^{l_d} u\right\|^2_{L^2(\mathbb{R}^d)}\right)^{\frac{1}{2}}.$$

According to [25], we have the following.

Lemma 6.1 *The previous three norms are equivalent, i.e.*,

$$\|u\|_{H^s_A(\mathbb{R}^d)} = \|u\|_{H^s_B(\mathbb{R}^d)} \sim \|u\|_{H^s_C(\mathbb{R}^d)}.$$

Remark 6.1 For $d=1$, we may also refer to [24].

Hereafter, let $d = 6\kappa + \kappa_0$ with integers $\kappa \geq 0$ and $0 \leq \kappa_0 \leq 5$. For convenience, we assume that

$$\begin{aligned} &\text{(i) if } \kappa_0 = 0, \text{ then } s_d = 5\kappa, && \text{(ii) if } \kappa_0 = 1, \text{ then } s_d = 5\kappa+1, \\ &\text{(iii) if } \kappa_0 = 2, 3, \text{ then } s_d = 5\kappa+2, && \text{(iv) if } \kappa_0 = 4,\ 5, \text{ then } s_d = 5\kappa+4. \end{aligned} \tag{6.6}$$

Lemma 6.2 *We have the following inequalities*:

$$\|uvw\|_{L^2(\mathbb{R}^d)} \leq c\|u\|_{H^{\frac{d}{3}}(\mathbb{R}^d)} \|v\|_{H^{\frac{d}{3}}(\mathbb{R}^d)} \|w\|_{H^{\frac{d}{3}}(\mathbb{R}^d)}, \tag{6.7}$$

$$\|uvw\|_{L^2(\mathbb{R}^d)} \leq c\|u\|_{L^2(\mathbb{R}^d)} \|v\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)} \|w\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}, \quad \forall \epsilon > 0, \tag{6.8}$$

$$\begin{aligned} &\|uvw\|_{H^k(\mathbb{R}^d)} \leq c\|u\|_{H^k(\mathbb{R}^d)} \|v\|_{H^{s_d}(\mathbb{R}^d)} \|w\|_{H^{s_d}(\mathbb{R}^d)}, \\ &\quad \forall \text{ integers } 1 \leq k < s_d, \end{aligned} \tag{6.9}$$

$$\begin{aligned} &\|uvw\|_{H^k(\mathbb{R}^d)} \leq c\|u\|_{H^k(\mathbb{R}^d)} \|v\|_{H^k(\mathbb{R}^d)} \|w\|_{H^k(\mathbb{R}^d)}, \\ &\quad \forall \text{ integers } k \geq s_d. \end{aligned} \tag{6.10}$$

Proof We proceed to treat different cases separately.

(i) The first bound follows from the Sobolev embedding $H^{\frac{d}{3}}(\mathbb{R}^d) \subset L^6(\mathbb{R}^d)$, and the second bound comes from the Sobolev embedding $H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$.

(ii) We now deal with (6.9). For simplicity, we denote

$$\partial_{\mathbf{x}}^l u = \sum_{l_1+\cdots+l_d=l} \partial_{x_1}^{l_1}\cdots\partial_{x_d}^{l_d} u.$$

(1) $1 \le k < \frac{d}{3}$. Since k is an integer number, we use (6.8) and (6.6) to deduce that for small enough $\epsilon > 0$,

$$\begin{aligned}\|uvw\|_{H^k(\mathbb{R}^d)} &\le \|u\|_{H^k(\mathbb{R}^d)}\|v\|_{H^{k+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\|w\|_{H^{k+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\\ &\le \|u\|_{H^k(\mathbb{R}^d)}\|v\|_{H^{s_d}(\mathbb{R}^d)}\|w\|_{H^{s_d}(\mathbb{R}^d)}.\end{aligned}$$

(2) $\frac{d}{3} \le k < s_d$. We consider the term $\|\partial_{\mathbf{x}}^l u \partial_{\mathbf{x}}^m v \partial_{\mathbf{x}}^n w\|_{L^2(\mathbb{R}^d)}$. It is clear that $l+m+n \le k$. Hence

(a) if $\max(m,n) < \frac{d}{3}$, then by (6.8) and (6.6), for small enough $\epsilon > 0$,

$$\begin{aligned}\left\|\partial_{\mathbf{x}}^l u \partial_{\mathbf{x}}^m v \partial_{\mathbf{x}}^n w\right\|_{L^2(\mathbb{R}^d)} &\le \|u\|_{H^l(\mathbb{R}^d)}\|v\|_{H^{m+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\|w\|_{H^{n+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\\ &\le \|u\|_{H^k(\mathbb{R}^d)}\|v\|_{H^{s_d}(\mathbb{R}^d)}\|w\|_{H^{s_d}(\mathbb{R}^d)}.\end{aligned}$$

(b) if $\frac{d}{3} \le \max(m,n) \le \frac{d}{2}$, then $l \le k - \frac{d}{3}$. Since m, n are integer numbers, we use (6.7) and (6.6) to obtain that

$$\begin{aligned}\left\|\partial_{\mathbf{x}}^l u \partial_{\mathbf{x}}^m v \partial_{\mathbf{x}}^n w\right\|_{L^2(\mathbb{R}^d)} &\le \|u\|_{H^{l+\frac{d}{3}}(\mathbb{R}^d)}\|v\|_{H^{m+\frac{d}{3}}(\mathbb{R}^d)}\|w\|_{H^{n+\frac{d}{3}}(\mathbb{R}^d)}\\ &\le \|u\|_{H^k(\mathbb{R}^d)}\|v\|_{H^{s_d}(\mathbb{R}^d)}\|w\|_{H^{s_d}(\mathbb{R}^d)}.\end{aligned}$$

(c) if $\max(m,n) > \frac{d}{2}$, for instance, $m > \frac{d}{2}$, then $l, n < k - \frac{d}{2}$. Therefore, by (6.8) we get that, for small enough $\epsilon > 0$,

$$\begin{aligned}\left\|\partial_{\mathbf{x}}^l u \partial_{\mathbf{x}}^m v \partial_{\mathbf{x}}^n w\right\|_{L^2(\mathbb{R}^d)} &\le \|u\|_{H^{l+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\|v\|_{H^m(\mathbb{R}^d)}\|w\|_{H^{n+\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\\ &\le \|u\|_{H^k(\mathbb{R}^d)}\|v\|_{H^{s_d}(\mathbb{R}^d)}\|w\|_{H^{s_d}(\mathbb{R}^d)}.\end{aligned}$$

A combination of the previous statements leads to the desired result.

(iii) It remains to consider (6.10). Clearly, the result (6.10) with $k = s_d$ can be proved in a similar fashion as before. Hence, by induction we obtain the result (6.10) with $k > s_d$. □

The previous results can be extended to the corresponding ones in $H_A^k(\mathbb{R}^d)$, as stated below.

Lemma 6.3 *The following inequalities hold*:

$$\|uvw\|_{L^2(\mathbb{R}^d)} \le c\|u\|_{H_A^{\frac{d}{3}}(\mathbb{R}^d)}\|v\|_{H_A^{\frac{d}{3}}(\mathbb{R}^d)}\|w\|_{H_A^{\frac{d}{3}}(\mathbb{R}^d)}, \tag{6.11}$$

$$\|uvw\|_{L^2(\mathbb{R}^d)} \le c\|u\|_{L^2(\mathbb{R}^d)}\|v\|_{H_A^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\|w\|_{H_A^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}, \quad \forall \epsilon > 0, \tag{6.12}$$

$$\|uvw\|_{H_A^k(\mathbb{R}^d)} \le c\|u\|_{H_A^k(\mathbb{R}^d)}\|v\|_{H_A^{s_d}(\mathbb{R}^d)}\|w\|_{H_A^{s_d}(\mathbb{R}^d)}, \quad \forall \text{ integers } 1 \le k < s_d, \tag{6.13}$$

$$\|uvw\|_{H_A^k(\mathbb{R}^d)} \le c\|u\|_{H_A^k(\mathbb{R}^d)}\|v\|_{H_A^k(\mathbb{R}^d)}\|w\|_{H_A^k(\mathbb{R}^d)}, \quad \forall \text{ integers } k \ge s_d. \tag{6.14}$$

Proof For simplicity, we only check the inequality (6.14). Clearly,

$$
\begin{aligned}
&\|uvw\|^2_{H^k_A(\mathbb{R}^d)}\\
&\quad\le c\|uvw\|^2_{H^k_C(\mathbb{R}^d)}\\
&\quad= c\sum_{l_1+\cdots+l_d=0}^{k}\Big\|\big(x_1^2+\cdots+x_d^2+1\big)^{\frac{k-l_1-\cdots-l_d}{2}}\partial_{x_1}^{l_1}\cdots\partial_{x_d}^{l_d}(uvw)\Big\|^2_{L^2(\mathbb{R}^d)}\\
&\quad= c\big\|\partial_{\mathbf{x}}^k(uvw)\big\|^2_{L^2(\mathbb{R}^d)}\\
&\qquad+c\sum_{l+m+n=0}^{k-1}\Big\|\big(x_1^2+\cdots+x_d^2+1\big)^{\frac{k-l-m-n}{2}}\partial_{\mathbf{x}}^l u\,\partial_{\mathbf{x}}^m v\,\partial_{\mathbf{x}}^n w\Big\|^2_{L^2(\mathbb{R}^d)}.
\end{aligned}
\tag{6.15}
$$

We next consider the term $\|(x_1^2+\cdots+x_d^2+1)^{\frac{k-l-m-n}{2}}\partial_{\mathbf{x}}^l u\partial_{\mathbf{x}}^m v\partial_{\mathbf{x}}^n w\|^2_{L^2(\mathbb{R}^d)}$. Without loss of generality, we assume that $l=\max(l,m,n)$. Since $l+m+n\le k-1$, we have that $m,n\le\frac{k-1}{3}$. Therefore, by (6.8) and the definition of the norm $\|\cdot\|_{H^k_C(\mathbb{R}^d)}$, a direct calculation shows that, for small enough $\epsilon>0$,

$$
\begin{aligned}
&\Big\|\big(x_1^2+\cdots+x_d^2+1\big)^{\frac{k-l-m-n}{2}}\partial_{\mathbf{x}}^l u\,\partial_{\mathbf{x}}^m v\,\partial_{\mathbf{x}}^n w\Big\|_{L^2(\mathbb{R}^d)}\\
&\quad\le\Big\|\big(x_1^2+\cdots+x_d^2+1\big)^{\frac{k-l-m-n}{2}}\partial_{\mathbf{x}}^l u\Big\|_{L^2(\mathbb{R}^d)}\big\|\partial_{\mathbf{x}}^m v\big\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\big\|\partial_{\mathbf{x}}^n w\big\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\\
&\quad\le\Big\|\big(x_1^2+\cdots+x_d^2+1\big)^{\frac{k-l}{2}}\partial_{\mathbf{x}}^l u\Big\|_{L^2(\mathbb{R}^d)}\big\|\partial_{\mathbf{x}}^m v\big\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\big\|\partial_{\mathbf{x}}^n w\big\|_{H^{\frac{d}{2}+\epsilon}(\mathbb{R}^d)}\\
&\quad\le\|u\|_{H^k_C(\mathbb{R}^d)}\|v\|_{H^k_C(\mathbb{R}^d)}\|w\|_{H^k_C(\mathbb{R}^d)}.
\end{aligned}
$$

Further, by (6.15), (6.10), the above inequality and the equivalence of the norms, we derive that

$$
\|uvw\|_{H^k_A(\mathbb{R}^d)}\le c\|u\|_{H^k_A(\mathbb{R}^d)}\|v\|_{H^k_A(\mathbb{R}^d)}\|w\|_{H^k_A(\mathbb{R}^d)}. \tag{6.16}
$$

□

Let us denote

$$
X_N=\operatorname{span}\big\{h_{l_1}(x_1)\cdots h_{l_d}(x_d):0\le l_1,\ldots,l_d\le N\big\}.
$$

For any $u\in L^2(\mathbb{R}^d)$, the orthogonal projection operator $P_N:L^2(\mathbb{R}^d)\to X_N$ is defined by

$$
(u-P_N u,\phi)_{\mathbb{R}^d}=0,\quad \forall\phi\in X_N. \tag{6.17}
$$

In particular, if $u\in H^s_B(\mathbb{R}^d)$ with integer $s\ge 0$, then we have

$$
\big(\mathcal{L}^{\frac{s}{2}}(u-P_N u),\mathcal{L}^{\frac{s}{2}}\phi\big)_{\mathbb{R}^d}=\big(u-P_N u,\mathcal{L}^s\phi\big)_{\mathbb{R}^d}=0,\quad\forall\phi\in X_N, \tag{6.18}
$$

which means that the $L^2(\mathbb{R}^d)$-orthogonal projection operator P_N is also the $H_B^s(\mathbb{R}^d)$-orthogonal projection operator.

We recall below an approximation result and an inverse inequality (cf. for instance [25]).

Lemma 6.4 *If* $u \in H_A^s(\mathbb{R}^d)$, *then for any* $0 \le \mu \le s$,

$$\|u - P_N u\|_{H_A^\mu(\mathbb{R}^d)} \le cN^{\frac{\mu-s}{2}} \|u\|_{H_A^s(\mathbb{R}^d)}.$$

Lemma 6.5 *For any* $\phi \in X_N$ *and* $s \ge 0$,

$$\|\phi\|_{H_A^s(\mathbb{R}^d)} \le cN^{\frac{s}{2}} \|\phi\|_{L^2(\mathbb{R}^d)}.$$

We now consider the interpolation operator. The Hermite–Gauss interpolant $\mathcal{I}_N : C(\mathbb{R}^d) \to X_N$ is determined by

$$\mathcal{I}_N u(z_{l_1}, \dots, z_{l_d}) = u(z_{l_1}, \dots, z_{l_d}), \quad 0 \le l_1, \dots, l_d \le N,$$

where $\{z_j\}$ are the Hermite–Gauss points. According to (2.11), we deduce readily that

$$\|\mathcal{I}_N u\|_{L^2(\mathbb{R}^d)} \le c \sum_{m=0}^{d} N^{-\frac{m}{6}} |u|_{H^m(\mathbb{R}^d)}, \tag{6.19}$$

where $|\cdot|_{H^m(\mathbb{R}^d)}$ denotes the seminorm of $H^m(\mathbb{R}^d)$. Hence, by a similar argument as in the proof of Theorem 2.2, we can prove the following result:

Theorem 6.1 *If* $u \in H_A^s(\mathbb{R}^d)$, *then for any* $0 \le \mu \le s$ *and* $s \ge d$,

$$\|u - \mathcal{I}_N u\|_{H_A^\mu(\mathbb{R}^d)} \le cN^{\frac{d}{3}+\frac{\mu-s}{2}} \|u\|_{H_A^s(\mathbb{R}^d)}.$$

Proof From Lemmas 6.4 and 6.5, for any $0 \le \mu \le s$,

$$\begin{aligned}\|u - \mathcal{I}_N u\|_{H_A^\mu(\mathbb{R}^d)} &\le \|u - P_N u\|_{H_A^\mu(\mathbb{R}^d)} + \left\|\mathcal{I}_N(u - P_N u)\right\|_{H_A^\mu(\mathbb{R}^d)} \\ &\le cN^{\frac{\mu-s}{2}} \|u\|_{H_A^s(\mathbb{R}^d)} + cN^{\frac{\mu}{2}} \left\|\mathcal{I}_N(u - P_N u)\right\|_{L^2(\mathbb{R}^d)}.\end{aligned}$$

Moreover, by (6.19) and Lemma 6.4, for any $s \ge d$,

$$\left\|\mathcal{I}_N(u - P_N u)\right\|_{L^2(\mathbb{R}^d)} \le c \sum_{m=0}^{d} N^{-\frac{m}{6}} \|u - P_N u\|_{H_A^m(\mathbb{R}^d)} \le cN^{\frac{d}{3}-\frac{s}{2}} \|u\|_{H_A^s(\mathbb{R}^d)}.$$

Therefore,

$$\|u - \mathcal{I}_N u\|_{H_A^\mu(\mathbb{R}^d)} \le cN^{\frac{d}{3}+\frac{\mu-s}{2}} \|u\|_{H_A^s(\mathbb{R}^d)}.$$

□

6.2 Error Bounds of the Semidiscretization in Time

In this section, we present error bounds for the semidiscretization in time t under the $H_A^k(\mathbb{R}^d)$-norms. The second-order Strang splitting in time for (6.1) is as follows:

$$\psi^{n+1} = \Phi^\tau\big(\psi^n\big) := \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}}\mathrm{e}^{-\mathrm{i}\tau|\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}}\psi^n|^2}\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}}\psi^n, \quad \psi^0 = \psi_0. \tag{6.20}$$

Since the error analysis for the above scheme is essentially the same as for the scheme (3.3), we shall present the results below without proof.

Lemma 6.6 (Stability) *If $\psi, \varphi \in H_A^{s_d}(\mathbb{R}^d) \cap H_A^k(\mathbb{R}^d)$ with integer $k \ge 0$, then we have*

$$\big\|\Phi^\tau(\psi) - \Phi^\tau(\varphi)\big\|_{H_A^k(\mathbb{R}^d)} \le \mathrm{e}^{c\tau(\|\psi\|^2_{H_A^j(\mathbb{R}^d)} + \|\varphi\|^2_{H_A^j(\mathbb{R}^d)})}\|\psi - \varphi\|_{H_A^k(\mathbb{R}^d)}, \tag{6.21}$$

where $j = \max(k, s_d)$.

Next, we denote

$$\widehat{T}(\psi) = -\mathrm{i}\mathcal{L}\psi, \qquad \widehat{V}(\psi) = -\mathrm{i}|\psi|^2\psi.$$

Their Lie commutator (cf. [12, 15]) is as follows:

$$[\widehat{T}, \widehat{V}](\psi) = \widehat{T}'(\psi)\widehat{V}(\psi) - \widehat{V}'(\psi)\widehat{T}(\psi) = -\mathcal{L}\big(|\psi|^2\psi\big) - \psi^2\mathcal{L}\overline{\psi} + 2|\psi|^2\mathcal{L}\psi.$$

Lemma 6.7 *If $\psi \in H_A^{k+2}(\mathbb{R}^d) \cap H_A^{s_d}(\mathbb{R}^d)$ with integer $k \ge 0$, then the commutator is bounded by*

$$\big\|[\widehat{T}, \widehat{V}](\psi)\big\|_{H_A^k(\mathbb{R}^d)} \le c\|\psi\|^3_{H_A^j(\mathbb{R}^d)}, \quad j = \max(k+2, s_d).$$

If, in addition, $\psi \in H_A^{k+4}(\mathbb{R}^d)$, then

$$\big\|\big[\widehat{T}, [\widehat{T}, \widehat{V}]\big](\psi)\big\|_{H_A^k(\mathbb{R}^d)} \le c\|\psi\|^3_{H_A^j(\mathbb{R}^d)}, \quad j = \max(k+4, s_d).$$

Lemma 6.8 (Local errors) *Let integer $k \ge 0$. If the exact solution $\psi(t) \in H_A^k(\mathbb{R}^d) \cap H_A^{s_d}(\mathbb{R}^d)$ for all $0 \le t \le \tau$, and $\psi_0 \in H_A^{k+2}(\mathbb{R}^d) \cap H_A^{s_d}(\mathbb{R}^d)$, then the local errors of the method (6.20) are bounded by*

$$\big\|\psi^1 - \psi(\tau)\big\|_{H_A^k(\mathbb{R}^d)} \le c\tau^2,$$

where c depends only on $\|\psi_0\|_{H_A^m(\mathbb{R}^d)}$ and $\max_{0\le t\le\tau}\|\psi\|_{H_A^j(\mathbb{R}^d)}$ with $m = \max(k+2, s_d)$ and $j = \max(k, s_d)$. If, in addition, $\psi_0 \in H_A^{k+4}(\mathbb{R}^d)$, then

$$\big\|\psi^1 - \psi(\tau)\big\|_{H_A^k(\mathbb{R}^d)} \le c\tau^3,$$

where c depends only on $\|\psi_0\|_{H_A^n(\mathbb{R}^d)}$ and $\max_{0\le t\le\tau}\|\psi\|_{H_A^j(\mathbb{R}^d)}$ with $n = \max(k+4, s_d)$.

Lemma 6.9 (Regularity of the numerical solution) *If the exact solution* $\psi(t) \in H_A^{k+2}(\mathbb{R}^d)$ *with integer* $k \geq s_d$ *and* $t \in [0, T]$, *then for small enough* τ *and any* $1 \leq n \leq N_0 = \frac{T}{\tau}$, *we have*

$$\max_{0 \leq j \leq N_0 - n} \left\| \left(\Phi^\tau\right)^n \left(\psi(j\tau)\right) \right\|_{H_A^k(\mathbb{R}^d)} \leq T + \max_{0 \leq t \leq T} \|\psi\|_{H_A^k(\mathbb{R}^d)}.$$

By using the above results and the same procedure as in the proof of Theorem 4.1, we can prove the following.

Theorem 6.2 *Suppose that integer* $k \geq 0$, τ *is small enough, and the exact solution* $\psi \in H_A^{k+2}(\mathbb{R}^d) \cap H_A^{s_d+2}(\mathbb{R}^d)$ *for all* $0 \leq t \leq T$. *Then, the solution of the scheme* (6.20) *satisfies*

$$\left\| \psi^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \leq c\tau, \quad t_n = n\tau \leq T,$$

where c *depends only on* T *and* $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^j(\mathbb{R}^d)}$ *with* $j = \max(k+2, s_d)$. *If, in addition,* $\psi(t) \in H_A^{k+4}(\mathbb{R}^d)$ *for all* $0 \leq t \leq T$, *then*

$$\left\| \psi^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \leq c\tau^2, \quad t_n = n\tau \leq T,$$

where c *depends only on* T *and* $\max_{0 \leq t \leq T} \|\psi(t)\|_{H_A^m(\mathbb{R}^d)}$ *with* $m = \max(k+4, s_d)$.

6.3 Error Bounds of the Full Discretization

The fully discrete Strang splitting Hermite collocation scheme for (6.1) is as follows:

$$\begin{aligned} &\psi_N^0 = \mathcal{I}_N \psi_0; \\ &\psi_N^{n+1} = \Phi_N^\tau\left(\psi_N^n\right) := \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}} \mathcal{I}_N \left(\mathrm{e}^{-\mathrm{i}\tau|\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}}\psi_N^n|^2} \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}\mathcal{L}} \psi_N^n\right), \quad n \geq 0. \end{aligned} \tag{6.22}$$

Then, by using a similar procedure as in the proofs of Lemma 5.1 and Theorem 5.1, we can prove the following.

Lemma 6.10 *If* $\psi \in X_N$ *and* $\varphi \in H_A^s(\mathbb{R}^d) \cap H_A^d(\mathbb{R}^d)$ *with integer* $s \geq s_d$, *then*

$$\begin{aligned} &\left\| \Phi_N^\tau(\psi) - P_N \Phi^\tau(\varphi) \right\|_{L^2(\mathbb{R}^d)}^2 \\ &\quad \leq \exp\left(c\tau \|\psi\|_{H_A^j(\mathbb{R}^d)} \|\varphi\|_{H_A^{s_d}(\mathbb{R}^d)} \exp\left(c\tau \|\varphi\|_{H_A^{s_d}(\mathbb{R}^d)}^2\right)\right) \|\psi - P_N \varphi\|_{L^2(\mathbb{R}^d)}^2 \\ &\qquad + c\tau^2 N^{\frac{d}{2}-s} \|\varphi\|_{H_A^d(\mathbb{R}^d)}^2 \|\varphi\|_{H_A^s(\mathbb{R}^d)}^4 \\ &\qquad \times \exp\left(c\tau \|\varphi\|_{H_A^m(\mathbb{R}^d)}^2 + c\tau \|\psi\|_{H_A^j(\mathbb{R}^d)} \|\varphi\|_{H_A^{s_d}(\mathbb{R}^d)} \exp\left(c\tau \|\varphi\|_{H_A^{s_d}(\mathbb{R}^d)}^2\right)\right), \end{aligned}$$

where $j = \frac{d}{2} + \epsilon$ *and* $m = \max(s, d)$.

Finally, with the above preparations and by using a similar argument as in the proof of Theorem 5.1, we can prove the following.

Theorem 6.3 *Let integer $s > \frac{7d}{6} - 2$ and $1 \le n \le \frac{T}{\tau}$. If the exact solution $\psi(t) \in H_A^{s+2}(\mathbb{R}^d)$ for all $0 \le t \le T$, then for N sufficiently large and τ sufficiently small, we have for $s-2 < k \le s$,*

$$\left\| \psi_N^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \le \begin{cases} cN^{\frac{d}{4}+\frac{k-s}{2}} + c\tau, & d < 12, s > d, \\ cN^{\frac{d}{3}-1+\epsilon+\frac{k-s}{2}} + c\tau, & d \ge 12, \forall \epsilon > 0, \end{cases} \tag{6.23}$$

and for $0 \le k \le s-2$,

$$\left\| \psi_N^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \le \begin{cases} cN^{\frac{d}{4}+\frac{k-s}{2}} + c\tau^2, & d < 12, s > d, \\ cN^{\frac{d}{3}-1+\epsilon+\frac{k-s}{2}} + c\tau^2, & d \ge 12, \forall \epsilon > 0. \end{cases} \tag{6.24}$$

As in the last section, the restriction on N in the above result can be removed if we replace $\psi_N^0 = \mathcal{I}_N \psi_0$ in (6.22) by $\psi_N^0 = P_N \psi_0$. More precisely, we can prove the following.

Corollary 6.1 *Let $\psi_N^0 = P_N \psi_0$ in (6.22). Then for integer $s > d$, $\psi(t) \in H_A^{s+2}(\mathbb{R}^d)$, $0 \le t \le T$, and τ sufficiently small, we have for $s-2 < k \le s$,*

$$\left\| \psi_N^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \le cN^{\frac{d}{4}+\frac{k-s}{2}} + c\tau, \quad 1 \le n \le \frac{T}{\tau}, \tag{6.25}$$

and for $0 \le k \le s-2$,

$$\left\| \psi_N^n - \psi(t_n) \right\|_{H_A^k(\mathbb{R}^d)} \le cN^{\frac{d}{4}+\frac{k-s}{2}} + c\tau^2, \quad 1 \le n \le \frac{T}{\tau}. \tag{6.26}$$

Remark 6.2 In Theorem 3.4 of [8], the author also presents a result under the $L^2(\mathbb{R}^d)$-norm, stated as follows: Let $s > [\frac{d+1}{2}] + 2 + \frac{2d}{3}$ be an even integer. If the exact solution $\psi(t) \in H_A^{s+2}(\mathbb{R}^d)$ for $0 \le t \le T$, then for N sufficiently large and τ sufficiently small,

$$\left\| \psi_N^n - \psi(t_n) \right\|_{L^2(\mathbb{R}^d)} \le cN^{1+\frac{d}{3}-\frac{s}{2}} + c\tau^2.$$

It is clear that the estimates in (6.24) are better both with respect to the order of convergence in space as well as the required regularity. In addition, the order of convergence and the regularity requirements of our results are further relaxed significantly if we replace $\psi_N^0 = \mathcal{I}_N \psi_0$ in (6.22) by $\psi_N^0 = P_N \psi_0$, as indicated in Corollary 6.1.

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Appendix: The Proof of Lemma 4.4

Proof The proof of Lemma 4.4 is analogous to the corresponding results for the Schrödinger–Poisson equation in [18]. For simplicity, we only verify (4.17). To this end, let $\widehat{H} = \widehat{T} + \widehat{V}$, and denote by D_H, D_T, and D_V the corresponding Lie derivatives (cf. [18]) of $\widehat{H}$, $\widehat{T}$, and $\widehat{V}$, respectively. According to Sect. 4.4 of [18],

$$\psi^1 - \psi(\tau) = \tau f\left(\frac{1}{2}\tau\right) - \int_0^\tau f(s)\,\mathrm{d}s + r_2 - r_1, \tag{A.1}$$

where $f(s) = \exp((\tau - s)D_T)D_V \exp(sD_T)\mathrm{Id}(\psi_0)$, Id is the identity operator, and

$$r_1 = \int_0^\tau \int_0^{\tau-s} \exp\big((\tau - s - \sigma)D_H\big)D_V \exp(\sigma D_T)D_V \exp(sD_T)\mathrm{Id}(\psi_0)\,\mathrm{d}\sigma\,\mathrm{d}s,$$

$$r_2 = \tau^2 \int_0^1 (1-\theta)\exp\left(\frac{1}{2}\tau D_T\right)\exp(\theta\tau D_V)D_V^2 \exp\left(\frac{1}{2}\tau D_T\right)\mathrm{Id}(\psi_0)\,\mathrm{d}\theta.$$

Next we write the principal error term in the second-order Peano form:

$$\tau f\left(\frac{1}{2}\tau\right) - \int_0^\tau f(s)\,\mathrm{d}s = \tau^3 \int_0^1 \nu(\theta) f''(\theta\tau)\,\mathrm{d}\theta$$

with the Peano kernel ν of the midpoint rule. We have (cf. Sect. 5.2 of [18])

$$\begin{aligned} f''(s) &= \exp\big((\tau - s)D_T\big)\big[D_T, [D_T, D_V]\big]\exp(sD_T)\mathrm{Id}(\psi_0) \\ &= \exp\big((\tau - s)D_T\big)D_{[\widehat{T},[\widehat{T},\widehat{V}]]}\exp(sD_T)\mathrm{Id}(\psi_0) \\ &= \mathrm{e}^{-is(\mathcal{A}_r+\mathcal{B}_z)}\big[\widehat{T}, [\widehat{T}, \widehat{V}]\big](\mathrm{e}^{-\mathrm{i}(\tau-s)(\mathcal{A}_r+\mathcal{B}_z)}\psi_0), \end{aligned}$$

where $[D_T, D_V] = D_T D_V - D_V D_T$. Hence by (4.14), the quadrature error is bounded in $H_A^k(\Omega)$ by $c\tau^3\|\psi_0\|^3_{H_A^{k+4}(\Omega)}$. Let us denote

$$g(s,\sigma) = \exp\big((\tau - s - \sigma)D_T\big)D_V \exp(\sigma D_T)D_V \exp(sD_T)\mathrm{Id}(\psi_0).$$

Then the remainder term can be expressed as

$$r_2 - r_1 = \frac{1}{2}\tau^2 g\left(\frac{1}{2}\tau, 0\right) - \int_0^\tau \int_0^{\tau-s} g(s,\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s + \widetilde{r}_2 - \widetilde{r}_1,$$

where

$$\widetilde{r}_1 = r_1 - \int_0^\tau \int_0^{\tau-s} g(s,\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s, \qquad \widetilde{r}_2 = r_2 - \frac{1}{2}\tau^2 g\left(\frac{1}{2}\tau, 0\right).$$

It is clear that (cf. [18])

$$\left\| \frac{1}{2}\tau^2 g\left(\frac{1}{2}\tau, 0\right) - \int_0^\tau \int_0^{\tau-s} g(s,\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \right\|_{H_A^k(\Omega)}$$

$$\leq c\tau^3\Big(\max_{0\leq s\leq\tau}\|\partial_s g\|_{H_A^k(\Omega)}+\max_{0\leq\sigma\leq\tau}\|\partial_\sigma g\|_{H_A^k(\Omega)}\Big).$$

By using a similar argument as in Sect. 5.2 of [18], we can obtain

$$\left\|\frac{1}{2}\tau^2 g\left(\frac{1}{2}\tau,0\right)-\int_0^\tau\int_0^{\tau-s} g(s,\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\right\|_{H_A^k(\Omega)}\leq c_1\tau^3,$$

where c_1 depends only on $\|\psi_0\|_{H_A^{k+2}(\Omega)}$.

Next, we estimate the term $\|\widetilde{r}_2\|_{H_A^k(\Omega)}$. By the Taylor expansion,

$$\exp(\theta\tau D_V)=I+\int_0^{\theta\tau}\exp(\xi D_V)D_V\,\mathrm{d}\xi=I+\theta\tau\int_0^1\exp(\theta\tau\varsigma D_V)D_V\,\mathrm{d}\varsigma,$$

whence

$$\widetilde{r}_2=\tau^3\int_0^1\int_0^1\theta(1-\theta)\exp\left(\frac{1}{2}\tau D_T\right)\exp(\theta\tau\varsigma D_V)D_V^3\exp\left(\frac{1}{2}\tau D_T\right)\mathrm{Id}(\psi_0)\,\mathrm{d}\varsigma\,\mathrm{d}\theta.$$

Setting $\phi=\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\psi_0$ and $\eta=\mathrm{e}^{-\mathrm{i}\theta\tau\varsigma\beta|\phi|^2}\phi$, a direct calculation shows that

$$\exp\left(\frac{1}{2}\tau D_T\right)\exp(\theta\tau\varsigma D_V)D_V^3\exp\left(\frac{1}{2}\tau D_T\right)\mathrm{Id}(\psi_0)=\mathrm{i}\beta^3\mathrm{e}^{-\mathrm{i}\frac{\tau}{2}(\mathcal{A}_r+\mathcal{B}_z)}\big(|\eta|^6\eta\big).$$

Hence, by (4.2)–(4.4) and (4.10), we find that for $j=\max(k,2)$,

$$\begin{aligned}&\left\|\exp\left(\frac{1}{2}\tau D_T\right)\exp(\theta\tau\varsigma D_V)D_V^3\exp\left(\frac{1}{2}\tau D_T\right)\mathrm{Id}(\psi_0)\right\|_{H_A^k(\Omega)}\\&\quad\leq c\|\eta\|^7_{H_A^j(\Omega)}\leq c_2\|\psi_0\|^7_{H_A^j(\Omega)},\end{aligned}$$

where c_2 depends only on $\|\psi_0\|_{H_A^j(\Omega)}$. Therefore, $\|\widetilde{r}_2\|_{H_A^k(\Omega)}\leq c_2\tau^3$.

It remains to estimate the term $\|\widetilde{r}_1\|_{H_A^k(\Omega)}$. By using the nonlinear variation-of-constants formula (cf. [18]), we obtain that

$$\begin{aligned}\widetilde{r}_1=&\int_0^\tau\int_0^{\tau-s}\int_0^{\tau-s-\sigma}\exp\big((\tau-s-\sigma-\xi)D_H\big)D_V\exp(\xi D_T)D_V\\&\times\exp(\sigma D_T)D_V\exp(sD_T)\mathrm{Id}(\psi_0)\,\mathrm{d}\xi\,\mathrm{d}\sigma\,\mathrm{d}s.\end{aligned}$$

By (4.2)–(4.4), a direct calculation gives

$$\begin{aligned}&\big\|\exp((\tau-s-\sigma-\xi)D_H)D_V\exp(\xi D_T)D_V\exp(\sigma D_T)D_V\exp(sD_T)\mathrm{Id}(\psi_0)\big\|_{H_A^k(\Omega)}\\&\quad\leq c\big\|\psi(\tau-s-\sigma-\xi)\big\|^7_{H_A^j(\Omega)},\qquad j=\max(k,2).\end{aligned}$$

Therefore, $\|\widetilde{r}_1\|_{H_A^k(\Omega)}\leq c_3\tau^3$, where c_3 depends only on $\max_{0\leq t\leq\tau}\|\psi\|_{H_A^j(\Omega)}$. A combination of the previous statements leads to (4.17). □

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