CONVERGENCE AND ENERGY CONSERVATION OF THE STRANG TIME-SPLITTING HERMITE SPECTRAL METHOD FOR NONLINEAR SCHRÖDINGER EQUATIONS*

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Abstract. In this paper, we consider nonlinear Schrödinger equations and deduce a second-order error bound for a Strang type time-splitting Hermite spectral method; furthermore, we study the energy conservation of the time discretisation. In particular, our analysis is applicable to the Gross–Pitaevskii equation

$$\mathrm{i}\,\hbar\,\partial_t\Psi(x,t) = \Big(-\tfrac{\hbar^2}{2\,m}\,\Delta + U(x) + \tfrac{4\pi\hbar^2 aN}{m}\,\big|\Psi(x,t)\big|^2\Big)\,\Psi(x,t)\,, \qquad x\in\mathbb{R}^d, \quad t\geq 0,$$

that arises in quantum physics as a mathematical model of a Bose–Einstein condensate. Numerical examples illustrate the theoretical results.

1. Introduction. In the present paper, we study the convergence behaviour and energy conservation of time-splitting Hermite spectral methods for nonlinear Schrödinger equations. Our main objective is to provide an error analysis for a Strang type [18, 23] time discretisation of the d-dimensional Gross–Pitaevskii equation (GPE)

$$\mathrm{i}\,\hbar\,\partial_t\Psi(x,t) = \Big(-\tfrac{\hbar^2}{2\,m}\,\Delta + U(x) + \tfrac{4\pi\hbar^2 aN}{m}\,\big|\Psi(x,t)\big|^2\Big)\,\Psi(x,t)\,; \tag{1.1}$$

the solution of (1.1) is subject to asymptotic boundary conditions on the unbounded domain and an initial condition. The GPE arises in quantum physics for the description of a Bose–Einstein condensate, see [10, 11, 17]; Ψ denotes the wave function of a boson in the condensate, $\hbar$ Planck's constant, m the mass of a boson, a its scattering length, N the total particle number, and U an external potential. We show that the Strang type time-splitting method retains its classical order for the GPE (1.1) involving a quasi-harmonic potential U, whenever Ψ fulfills suitable regularity requirements.

Due to their favourable properties regarding accuracy, efficiency, and geometric behaviour, time-splitting spectral methods are widely used for the numerical solution of nonlinear Schrödinger equations; we refer the reader to the works [2, 3, 4, 5, 9, 16, 20, 19, 22, 24] and the references therein; see also [12, 15] for detailed information on splitting methods. However, so far, it remains open to provide a convergence analysis of high-order splitting methods when applied to stiff nonlinear problems.

For linear evolutionary Schrödinger equations, a second-order error estimate for the Strang time-splitting Fourier pseudo-spectral method is proven in Jahnke and Lubich [13]; in Thalhammer [21], a stability and convergence analysis is given for exponential operator splitting methods of arbitrary order. The recent work Lubich [14] is concerned with error bounds for a Strang type time-splitting Fourier spectral method when applied to the Schrödinger–Poisson and the cubic nonlinear Schrödinger equation, respectively.

In the present paper, we extend the approach of [13, 14, 21] and provide a stability and convergence result for Strang type time-splitting Hermite spectral discretisations

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of nonlinear Schrödinger equations; moreover, we deduce a bound for the drift in the energy. The considered numerical scheme is defined by four coefficients, which we assume to satisfy the classical second-order conditions. In particular, our analysis is applicable to the Gross–Pitaevskii equation (1.1) involving an unbounded harmonic potential. Our proofs primarily rely on elementary techniques; we employ a Hermite spectral decomposition, the (linear) variation-of-constants formula, and, of course, taylor series expansions; further, results from functional analysis such as continuous embeddings are needed. For the convenience of the reader, several standard results are reviewed in an appendix.

The present paper is organised as follows. We start by introducing several auxiliary abbreviations employed throughout, see Section 1.1. In Sections 2 and 3, we restate the GPE (1.1) in a normalised form and further specify the time discretisation; for the latter, it is convenient to rewrite the partial differential equation as an abstract evolution equation. Our main results, a second-order error estimate with respect to the norm of the Sobolev space $H^m\big(\mathbb{R}^d\big)$ and a bound for the error in the energy are given in Section 4. Their proofs rely on a stability estimate and an expansion of the local error; these auxiliary results are deduced in Sections 5 and 6. Additional considerations are collected in the appendix.

1.1. Notations. In addition to standard notations, we henceforth tacitly employ the following abbreviations, see also [1, 25].

For a multi-index $\mu = (\mu_1, \dots, \mu_d) \in \mathbb{Z}^d$, the relation $\geq$ is defined componentwise; furthermore, we set $|\mu| = \mu_1 + \cdots + \mu_d$. Partial derivatives with respect to $\xi = (\xi_1, \dots, \xi_d) \in \mathbb{R}^d$ are denoted by $\partial^\mu = \partial_{\xi_1}^{\mu_1} \dots \partial_{\xi_d}^{\mu_d}$.

For any $1 \leq p \leq \infty$, the Lebesgue space $L^p\big(\mathbb{R}^d\big) = L^p\big(\mathbb{R}^d, \mathbb{C}\big)$ is a Banach space with associated norm $\|\cdot\|_{L^p}$ given by

$$\|f\|_{L^p} = \bigg(\int_{\mathbb{R}^d} \big|f(\xi)\big|^p \,\mathrm{d}\xi\bigg)^{\frac{1}{p}}, \quad 1 \leq p < \infty, \qquad \|f\|_{L^\infty} = \operatorname*{ess\,sup}_{\xi \in \mathbb{R}^d} \big|f(\xi)\big| . \tag{1.2a}$$

The Sobolev space $W^{m,p}\big(\mathbb{R}^d\big)$ comprises all functions with partial derivatives up to order $m \geq 0$ contained in $L^p\big(\mathbb{R}^d\big)$; $W^{m,p}\big(\mathbb{R}^d\big)$ is endowed with the norm

$$\|f\|_{W^{m,p}} = \sum_{\mu \geq 0,\, |\mu| \leq m} \big\|\partial^\mu f\big\|_{L^p}, \qquad f \in W^{m,p}\big(\mathbb{R}^d\big) . \tag{1.2b}$$

In particular, we set $H^m\big(\mathbb{R}^d\big) = W^{m,2}\big(\mathbb{R}^d\big)$; we recall that the scalar product

$$(f\,|\,g)_{L^2} = \int_{\mathbb{R}^d} f(\xi)\,\overline{g(\xi)}\,\mathrm{d}\xi, \qquad f, g \in L^2\big(\mathbb{R}^d\big),$$

renders $H^0\big(\mathbb{R}^d\big) = L^2\big(\mathbb{R}^d\big)$ a Hilbert space. In view of our convergence result, we introduce the subspace

$$D_{m,k}\big(\mathbb{R}^d\big) = \Big\{ v \in H^{m+k}\big(\mathbb{R}^d\big) : \Xi_\ell^{(k)} v \in H^m\big(\mathbb{R}^d\big) \text{ for } 1 \leq \ell \leq d \Big\}, \tag{1.3}$$

where $\Xi_\ell^{(k)}(\xi) = \xi_\ell^k$ and thus $\big(\Xi_\ell^{(k)} v\big)(\xi) = \xi_\ell^k\, v(\xi)$. The space of m-times continuously differentiable functions is denoted by $\mathscr{C}^m\big(\mathbb{R}^d\big)$; $\mathscr{C}_B^m\big(\mathbb{R}^d\big)$ comprises all functions in $\mathscr{C}^m\big(\mathbb{R}^d\big)$ with bounded derivatives up to order m.

The product of operators $K_j : H^m(\mathbb{R}^d) \to H^m(\mathbb{R}^d)$, $1 \leq j \leq J$, is defined downwards

$$\prod_{j=1}^{J} K_j = K_J \cdots K_1\,, \quad J \geq 1\,, \qquad \prod_{j=1}^{J} K_j = I\,, \quad J < 1\,;$$

here, I denotes the identity operator on $H^m(\mathbb{R}^d)$. In view of our convergence proof, it is also convenient to introduce the functions $\varphi_j : \mathbb{C} \to \mathbb{C}$ that are related to the exponential

$$\varphi_0(z) = \mathrm{e}^z, \qquad \varphi_j(z) = \tfrac{1}{(j-1)!} \int_0^1 \tau^{j-1}\, \mathrm{e}^{(1-\tau)z}\, \mathrm{d}\tau, \quad j \geq 1, \qquad z \in \mathbb{C}\,; \tag{1.4a}$$

by means of partial integration the recurrence relation

$$\varphi_j(z) = \tfrac{1}{j!} + z\, \varphi_{j+1}(z)\,, \qquad j \geq 0\,, \quad z \in \mathbb{C}\,, \tag{1.4b}$$

follows.

If not stated otherwise, we do not distinguish the arising constants and denote by C a generic constant.

2. Nonlinear Schrödinger equations. In this paper, we study in detail the error behaviour of a Strang type time-splitting method when applied to the Gross–Pitaevskii equation. As regards existence and regularity results for nonlinear evolutionary Schrödinger equations, we refer the reader to Cazenave [8].

2.1. Gross–Pitaevskii equation. We consider the d-dimensional GPE (1.1) on the unbounded domain, subject to asymptotic boundary conditions and an initial condition; throughout, we employ the following normalised form of the equation

$$\begin{gathered} \mathrm{i}\,\partial_t \psi(\xi,t) = \Big(-\tfrac{1}{2}\,\Delta_\gamma + V(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2 \Big)\, \psi(\xi,t)\,, \qquad \xi \in \mathbb{R}^d, \quad t \geq 0\,, \\ \Delta_\gamma = \sum_{j=1}^{d} \gamma_j\, \partial_{\xi_j}^2\,, \qquad \gamma_j > 0\,, \quad 1 \leq j \leq d\,, \end{gathered} \tag{2.1a}$$

see Section B.1. Here, we assume $V : \mathbb{R}^d \to \mathbb{R}$ to be a quasi-harmonic real potential, that is, the following decomposition

$$V = \tfrac{1}{2}\, V_\gamma + W\,, \qquad V_\gamma(\xi) = \sum_{j=1}^{d} \gamma_j\, \xi_j^2\,, \tag{2.1b}$$

is valid with a sufficiently regular function W; more precisely, for some integer $m \geq 0$ we suppose $\partial^\mu W \in L^\infty(\mathbb{R}^d)$ for $|\mu| \leq m$. Moreover, we require $\vartheta > 0$.

In order to introduce time-splitting methods for (2.1), it is useful to formulate the partial differential equation as an abstract evolution equation for $u(t) = \psi(\cdot,t)$

$$\begin{gathered} u'(t) = \Big(A + B\big(u(t)\big) \Big)\, u(t)\,, \qquad t \geq 0\,, \\ A = -\tfrac{1}{2}\,\mathrm{i}\,\big(-\Delta_\gamma + V_\gamma \big)\,, \qquad B(v) = -\,\mathrm{i}\,\big(W + \vartheta\,|v|^2 \big)\,. \end{gathered} \tag{2.2a}$$

We note that the linear operator $A : D_{m,2}(\mathbb{R}^d) \to H^m(\mathbb{R}^d)$ is well-defined, see (1.3). On the other hand, provided that $v \in H^j(\mathbb{R}^d)$ with integer j given by

$$\begin{aligned} &j = 1 \quad \text{if } d = 1\,,\ m = 0\,, && j = m \quad \text{if } d = 1\,,\ m \geq 1\,, \\ &j = 2 \quad \text{if } d = 2,3\,,\ m = 0,1\,, && j = m \quad \text{if } d = 2,3\,,\ m \geq 2\,, \end{aligned} \tag{2.2b}$$

it is ensured that the multiplication operator $B(v) : H^m(\mathbb{R}^d) \to H^m(\mathbb{R}^d)$ is well-defined; this is a consequence of the continuous embeddings $H^1(\mathbb{R}) \subset L^\infty(\mathbb{R})$ as well as $H^1(\mathbb{R}^d) \subset L^6(\mathbb{R}^d)$ and $H^2(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$ for $d = 2, 3$, see also Appendix B.3.

2.2. Particle number and energy conservation. For nonlinear Schrödinger equations such as (2.1), the particle number $\|\psi(\cdot, t)\|_{L^2}^2$ is a conserved quantity; thus, it holds $\|\psi(\cdot, t)\|_{L^2}^2 = \|\psi(\cdot, 0)\|_{L^2}^2$ for any $t \geq 0$, see Appendix B.2. Moreover, for the GPE (2.1), the energy functional is given by

$$E\big(\psi(\cdot, t)\big) = \Big(\Big(- \tfrac{1}{2}\, \Delta_\gamma + V + \tfrac{1}{2}\, \vartheta \, \big|\psi(\cdot, t)\big|^2\Big) \psi(\cdot, t) \,\Big|\, \psi(\cdot, t)\Big)_{L^2} ; \tag{2.3}$$

as shown in Appendix B.2, the energy functional is time-independent, that is, the relation $E\big(\psi(\cdot, t)\big) = E\big(\psi(\cdot, 0)\big)$ remains valid for $t \geq 0$.

3. Exponential operator splitting spectral methods. For the numerical solution of time-dependent Schrödinger equations, exponential operator splitting spectral methods are widely used; in particular, for the GPE, the favourable behaviour of time-splitting pseudospectral methods has been confirmed in the recent works [2, 3, 4, 7, 9, 19, 22], see also references given therein.

In the present paper, our objective is to provide a convergence analysis of a second-order Strang type time-splitting method for (2.2). For detailed information on a spatial discretisation of (2.1) by the Hermite spectral method, we refer to [6, 7]; several fundamental properties of the Hermite basis functions $(\mathscr{H}_\mu)$ with associated eigenvalues (λ_μ) are also collected in Appendix A.

3.1. Strang type time-splitting methods. Exponential operator splitting methods for (2.1) and (2.2), respectively, rely on the fact that the initial value problems

$$v'(t) = A\, v(t)\,, \quad t \geq 0\,, \qquad v(0) \text{ given}\,, \tag{3.1a}$$

$$w'(t) = B\big(w(t)\big)\, w(t)\,, \quad t \geq 0\,, \qquad w(0) \text{ given}\,, \tag{3.1b}$$

can be solved numerically in an accurate and efficient way. On the one hand, employing a Hermite spectral decomposition of the initial value, it follows

$$v(t) = \mathrm{e}^{tA}\, v(0) = \sum_\mu v_\mu\, \mathrm{e}^{-\,\mathrm{i}\, t\, \lambda_\mu}\, \mathscr{H}_\mu\,, \quad t \geq 0\,, \qquad v(0) = \sum_\mu v_\mu\, \mathscr{H}_\mu\,, \tag{3.1c}$$

see Appendix A. For a practical realisation of (3.1c), we truncate the infinite sum and compute the coefficients v_μ by means of the Gauss–Hermite quadrature formula; further, we collocate the equation at the Gauss–Hermite quadrature nodes. On the other hand, making use of the fact that the relation $B\big(w(t)\big) = B\big(w(0)\big)$ holds for the solution of (3.1b), see Appendix B.2, we obtain

$$w(t) = \mathrm{e}^{tB(w(0))}\, w(0)\,; \tag{3.1d}$$

as before, we collocate the equation at the Gauss–Hermite quadrature nodes.

We are now ready to state the time integration scheme for (2.2). For a constant time-step $h > 0$ and a starting value u_0, a numerical approximation u_n to the exact solution value $\widehat{u}_n = u(t_n)$ at time $t_n = nh$ is given by the recurrence relation

$$\begin{gathered} U_{n1} = \mathrm{e}^{a_1 hA}\, u_{n-1}\,, \qquad U_{n2} = \mathrm{e}^{a_2 hA}\, \mathrm{e}^{b_1 hB(U_{n1})}\, U_{n1}\,, \\ u_n = \mathrm{e}^{b_2 hB(U_{n2})}\, U_{n2}\,, \qquad n \geq 1\,, \end{gathered} \tag{3.2a}$$

involving the real method coefficients $a_j, b_j \in \mathbb{R}$, $j = 1, 2$. For instance, we choose $a_1 = \frac{1}{2} = a_2$, $b_1 = 1$, $b_2 = 0$ and $a_1 = 0$, $a_2 = 1$, $b_1 = \frac{1}{2} = b_2$, respectively; in both cases, the conditions for order two

$$a_1 + a_2 = 1\,, \qquad b_1 + b_2 = 1\,, \qquad b_1 a_1 + b_2 = \tfrac{1}{2}\,, \tag{3.2b}$$

are fulfilled.

We note that the numerical solution u_n remains well-defined in $H^m\big(\mathbb{R}^d\big)$, provided that the initial value u_0 and the potential W satisfy suitable regularity requirements. More precisely, for $d = 1$, $m \geq 1$, and for $d = 2, 3$, $m \geq 2$, respectively, we require u_0 to be bounded in $H^m\big(\mathbb{R}^d\big)$ and $\partial^\mu W \in L^\infty\big(\mathbb{R}^d\big)$ for $|\mu| \leq m$; then, the bounds

$$\begin{gathered}\big\|\mathrm{e}^{tA}\big\|_{H^m \leftarrow H^m} = 1\,, \quad \big\|\mathrm{e}^{t\,B(v)}\big\|_{H^m \leftarrow H^m} \leq \mathrm{e}^{C_1(m,v)\,t}\,, \qquad t \geq 0\,, \\ C_1(m, v) = C\,\Big(\max_{|\mu| \leq m} \big\|\partial^\mu W\big\|_{L^\infty} + \vartheta\,\|v\|_{H^m}^2\Big)\,,\end{gathered}$$

ensure that u_n remains bounded in $H^m\big(\mathbb{R}^d\big)$ for all $n \geq 1$, see Lemma 1-2 and (B.4). Otherwise, for $d = 1$, $m = 0$, and $d = 2, 3$, $m = 0, 1$, respecively, we assume u_0 to be bounded in $H^j\big(\mathbb{R}^d\big)$ and $\partial^\mu W \in L^\infty\big(\mathbb{R}^d\big)$ for $|\mu| \leq j$ with j given by (2.2b); then, the numerical solution is bounded in $H^j\big(\mathbb{R}^d\big)$ and in particular in $H^m\big(\mathbb{R}^d\big)$.

4. Convergence and energy conservation. In this section, we state our main result, a second-order error estimate for the time-splitting scheme (3.2) when applied to the GPE (2.2), and further a result concerning the energy conservation.

For the following considerations, it is convenient to introduce the nonlinear solution operator $\mathscr{E}$ and the splitting operator $\mathscr{S}$ that is defined by (3.2a)

$$\widehat{u}_n = \mathscr{E}(\widehat{u}_{n-1})\,, \qquad u_n = \mathscr{S}(u_{n-1})\,, \qquad n \geq 1\,; \tag{4.1}$$

we recall that the exact solution values are denoted by $\widehat{u}_n = u(t_n)$.

4.1. Convergence. In order to prove a convergence estimate for (3.2), we proceed as follows. By means of a Lady Windermere fan argument, that is, by adding and substracting $\mathscr{S}^\ell(\widehat{u}_{n-\ell})$ for $0 \leq \ell \leq n$, we obtain the following identity for the global error

$$\begin{aligned}u_n - \widehat{u}_n &= \mathscr{S}^n(u_0) - \mathscr{S}^n(\widehat{u}_0) \\ &\quad - \sum_{\ell=0}^{n-1} \Big(\mathscr{S}^\ell\big(\mathscr{E}(\widehat{u}_{n-\ell-1})\big) - \mathscr{S}^\ell\big(\mathscr{S}(\widehat{u}_{n-\ell-1})\big)\Big)\,, \qquad n \geq 0\,.\end{aligned} \tag{4.2}$$

In Section 5, we first derive a stability result for the Strang type splitting method (3.2) that implies the bound

$$\big\|\mathscr{S}^\ell(v) - \mathscr{S}^\ell(\widetilde{v})\big\|_{H^m} \leq C\,\|v - \widetilde{v}\|_{H^m} \tag{4.3a}$$

with a constant C depending in particular on the quantities $\|v\|_{H^j}$, $\|\widetilde{v}\|_{H^j}$, t_ℓ, ϑ, and on $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j\big\}$, see (2.2b) for the definition of j. Section 6 is then concerned with a suitable expansion of the local error yielding

$$\big\|\mathscr{E}(\widehat{u}_\ell) - \mathscr{S}(\widehat{u}_\ell)\big\|_{H^m} \leq C\,h^3\,, \qquad 0 \leq \ell \leq n-1; \tag{4.3b}$$

here, we require $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j+4\big\}$ and $\max\big\{\|u(t)\|_{D_{j,4}} : 0 \leq t \leq t_n\big\}$ to be bounded. Estimating (4.2) by means of the above estimates (4.3), we obtain the following convergence result.

THEOREM 1. *For some $m \geq 0$ let j be defined through* (2.2b). *Suppose that* $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j+4\big\}$, $\max\big\{\|u(t)\|_{D_{j,4}} : 0 \leq t \leq t_n\big\}$, *and* $\|u_0\|_{H^j}$ *are bounded. Then, the Strang type splitting method* (3.2), *when applied to the nonlinear Schrödinger equation* (2.2), *satisfies the convergence estimate*

$$\big\|u_n - \widehat{u}_n\big\|_{H^m} \leq C\left(\big\|u_0 - \widehat{u}_0\big\|_{H^m} + h^2\right), \qquad n \geq 0,$$

with a constant C which in particular depends on t_n and ϑ.

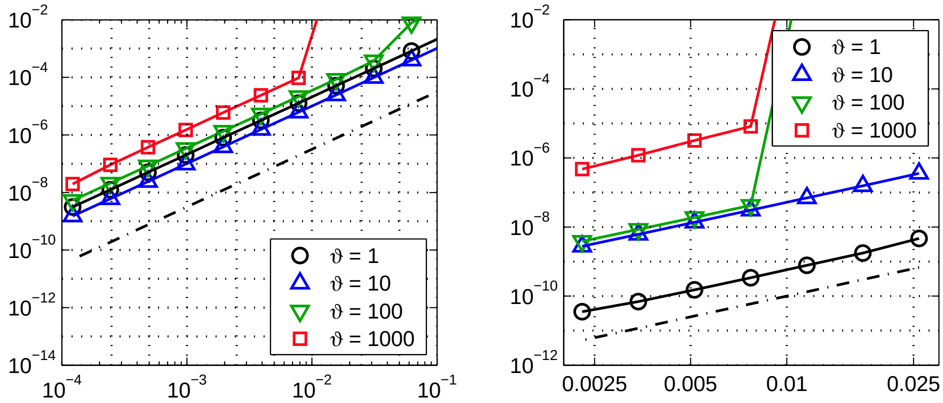

FIG. 4.1. *Left picture: Temporal order of a Strang type time-splitting Hermite spectral method when applied to the one-dimensional GPE with $V(\xi) = \frac{1}{2}\,\xi^2 + \cos(2\,\xi)$. Error versus stepsize. Right picture: Energy drift of a Strang type time-splitting Hermite spectral method when applied to the one-dimensional GPE with harmonic potential. Error versus stepsize.*

The above convergence result is illustrated by a numerical example for the one-dimensional GPE involving the quasi-harmonic potential $V(\xi) = \frac{1}{2}\,\xi^2 + \cos(2\,\xi)$. For the space and time discretisation of (2.1), we choose 256 Hermite basis functions and time stepsizes ranging from 2^{-13} to 2^{-4}. In order to determine the convergence order of the Strang type splitting method (3.2) with $a_1 = 0$, $a_2 = 1$, and $b_1 = \frac{1}{2} = b_2$, we consider the time evolution of the ground state solution up to a final time $t_n = 1$. For various values of the paramterer ϑ, the numerically obtained temporal convergence orders with respect to the norm of $L^2(\mathbb{R}^d)$ are displayed in Figure 4.1 (left picture); the slope of the dashed-dotted line is the expected convergence order two. We refer to CALIARI AND THALHAMMER [7] for further details on the implementation.

4.2. Energy conservation. The energy functional E associated with (2.2) is given by

$$\begin{aligned} &E(v) = \Big(\big(\widetilde{A} + \widetilde{B}(v)\big)\, v \,\Big|\, v\Big)_{L^2}\,, \\ &\widetilde{A} = \tfrac{1}{2}\big(-\Delta_\gamma + V_\gamma\big)\,, \qquad \widetilde{B}(v) = W + \tfrac{1}{2}\,\vartheta\,|v|^2\,. \end{aligned} \tag{4.4}$$

see also (2.1) and (2.3). As shown in Appendix B.2, the energy is conserved in (2.2), that is, for any initial value $v \in L^2(\mathbb{R}^d)$ it holds

$$E\big(\mathscr{E}^\ell(v)\big) = E(v)\,, \qquad \ell \geq 0\,; \tag{4.5}$$

the nonlinear solution operator $\mathscr{E}$ is introduced in (4.1). In order to estimate the defect of the numerical solution $E(u_n) - E(\widehat{u}_0)$, we add and substract $E\big(\mathscr{E}^\ell(u_{n-\ell})\big)$

	$t_n = 1$	$t_n = 2$	$t_n = 4$	$t_n = 8$	$t_n = 16$
$\vartheta = 1$	$0.7 \cdot 10^{-12}$	$1.4 \cdot 10^{-12}$	$2.8 \cdot 10^{-12}$	$5.7 \cdot 10^{-12}$	$11.3 \cdot 10^{-12}$
$\vartheta = 10$	$0.6 \cdot 10^{-11}$	$1.2 \cdot 10^{-11}$	$2.4 \cdot 10^{-11}$	$4.8 \cdot 10^{-11}$	$9.6 \cdot 10^{-11}$
$\vartheta = 100$	$0.9 \cdot 10^{-11}$	$1.8 \cdot 10^{-11}$	$3.7 \cdot 10^{-11}$	$7.3 \cdot 10^{-11}$	$14.6 \cdot 10^{-11}$
$\vartheta = 1000$	$0.1 \cdot 10^{-10}$	$0.3 \cdot 10^{-10}$	$0.6 \cdot 10^{-10}$	$1.2 \cdot 10^{-10}$	$2.5 \cdot 10^{-10}$

TABLE 4.1

Energy drift of a Strang type time-splitting Hermite spectral method when applied to the one-dimensional GPE with harmonic potential. Dependence on the final time t_n.

for $0 \leq \ell \leq n-1$; this yields

$$E(u_n) - E(\widehat{u}_0) = E\big(u_0\big) - E(\widehat{u}_0) + \sum_{\ell=0}^{n-1} E\big(\mathscr{E}^{\ell}(u_{n-\ell})\big) - E\big(\mathscr{E}^{\ell+1}(u_{n-\ell-1})\big)\,.$$

Further, by applying relation (4.5) and $u_{n-\ell} = \mathscr{S}(u_{n-\ell-1})$, we obtain

$$E(u_n) - E(\widehat{u}_0) = E\big(u_0\big) - E(\widehat{u}_0) + \sum_{\ell=0}^{n-1} E\big(\mathscr{S}(u_{n-\ell-1})\big) - E\big(\mathscr{E}(u_{n-\ell-1})\big)\,, \qquad (4.6)$$

see also (4.1). A brief calculation yields the relation

$$\begin{aligned} E(v) - E(w) = {}& \big(\widetilde{A}\,(v-w)\,\big|\,v\big)_{L^2} + \Big(\widetilde{A}\,w\,\Big|\,v-w\Big)_{L^2} \\ &+ \Big(\widetilde{B}(v)\,v - \widetilde{B}(w)\,w\,\Big|\,v\Big)_{L^2} + \Big(\widetilde{B}(w)\,w\,\Big|\,v-w\Big)_{L^2}\,, \end{aligned}$$

where $\widetilde{B}(v)\,v - \widetilde{B}(w)\,w = W(v-w) + \frac{1}{2}\,\vartheta\,\big(|v|^2 + \overline{v}\,w\big)\,(v-w) + \frac{1}{2}\,\vartheta\,w^2\,\overline{(v-w)}$, see (4.4). Similar considerations as in Section B.3 and the inequality of Cauchy–Schwarz thus imply the estimate

$$\big|E(v) - E(w)\big| \leq C\,\|v-w\|_{D_{0,1}} \qquad (4.7)$$

with a constant C depending in particular on $\|W\|_{L^\infty}$, $\|v\|_{D_{0,1}}$, $\|w\|_{D_{0,1}}$, and ϑ, see also (1.3). We note that $\mathscr{S}(v) \in H^j\big(\mathbb{R}^d\big) \cap D_{0,1}\big(\mathbb{R}^d\big)$ provided that $v \in H^j\big(\mathbb{R}^d\big) \cap D_{0,1}$ and $\partial^\mu W \in L^\infty\big(\mathbb{R}^d\big)$ for $|\mu| \leq j$ with j defined by (2.2b) for $m = 0$. Moreover, provided that $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j+4\big\}$ and $\max\big\{\|u(t)\|_{D_{j,4}} : 0 \leq t \leq t_n\big\}$ are bounded, the analogue of the local error estimate (6.8) is valid in $D_{0,1}\big(\mathbb{R}^d\big)$. As a consequence, by applying the above bound (4.7) to (4.6), we obtain the following result.

THEOREM 2. *Let $j = 1$ if $d = 1$ and $j = 2$ if $d = 2, 3$, respectively. Suppose that $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j+4\big\}$, $\max\big\{\|u(t)\|_{D_{j,4}} : 0 \leq t \leq t_n\big\}$, and $\max\big\{\|u_0\|_{H^j}, \|u_0\|_{D_{0,1}}\big\}$ are bounded. Then, the estimate*

$$\big|E(u_n) - E(\widehat{u}_0)\big| \leq C\Big(\big\|u_0 - \widehat{u}_0\big\|_{H^j} + \big\|u_0 - \widehat{u}_0\big\|_{D_{0,1}} + t_n\,h^2\Big), \qquad n \geq 0, \qquad (4.8)$$

is valid for the Strang type splitting method (3.2); the constant C in particular depends on ϑ.

In order to illustrate Theorem 2, we consider the GPE (2.1) in one space dimension with harmonic potential $V = V_\gamma$; similarly to before, for different values of ϑ, we integrate the ground state solution up to $t_n = 1$ by the Strang type splitting method (3.2) with 256 Hermite basis functions and time stepsizes ranging from $1.5\cdot 10^{-3}$ to $2\cdot 10^{-2}$. The energy drift $|E(u_n)-E(\widehat{u}_0)|$ is displayed in Figure 4.1 (right picture); the dashed-dotted line corresponds to the expected slope two. The linear dependence of the above bound (4.8) on the final time t_n is confirmed by Table 4.1, where we display the quantity $|E(u_n) - E(\widehat{u}_0)|$ for $t_n = 2^j$, $0 \leq j \leq 4$, and a fixed time stepsize $h = 2^{-10}$; in accordance with the theoretical result the energy drift increases by a factor two.

5. Stability. In this section, we are concerned with deriving a stability result for the Strang type splitting method (3.2); to this end, we consider

$$\begin{aligned}
&\mathscr{S}(v_{n-1}) = \mathrm{e}^{b_2 h B(V_{n2})}\, V_{n2}\,, \qquad V_{n2} = \mathrm{e}^{a_2 h A}\, \mathrm{e}^{b_1 h B(V_{n1})}\, V_{n1}\,, \qquad V_{n1} = \mathrm{e}^{a_1 h A}\, v_{n-1}\,,\\
&\mathscr{S}(\widetilde{v}_{n-1}) = \mathrm{e}^{b_2 h B(\widetilde{V}_{n2})}\, \widetilde{V}_{n2}\,, \qquad \widetilde{V}_{n2} = \mathrm{e}^{a_2 h A}\, \mathrm{e}^{b_1 h B(\widetilde{V}_{n1})}\, \widetilde{V}_{n1}\,, \qquad \widetilde{V}_{n1} = \mathrm{e}^{a_1 h A}\, \widetilde{v}_{n-1}\,.
\end{aligned}$$

With the help of the bounds for e^{tA} and $\mathrm{e}^{tB(v)}$ that are given in Appendix B.3, we are able to prove the following result.

THEOREM 3. *Suppose v_{n-1} and $\widetilde{v}_{n-1}$ to be bounded in $H^j(\mathbb{R}^d)$ and assume $\partial^\mu W \in L^\infty(\mathbb{R}^d)$ for $|\mu| \leq j$, where j is given by* (2.2b). *Then, the bound*

$$\big\|\mathscr{S}(v_{n-1}) - \mathscr{S}(\widetilde{v}_{n-1})\big\|_{H^m} \leq \mathrm{e}^{C_4 h}\, \|v_{n-1} - \widetilde{v}_{n-1}\|_{H^m}$$

holds with constant $C_4 = |b_1|\, C_3(m, V_{n1}, \widetilde{V}_{n1}) + |b_2|\, C_3(m, V_{n2}, \widetilde{V}_{n2})$, see Lemma 2 and 3 for the definition of C_3; in particular, the quantitity C_4 depends on $\|v_{n-1}\|_{H^j}$, $\|\widetilde{v}_{n-1}\|_{H^j}$, ϑ, and $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \leq j\big\}$.

Proof. In order to estimate $\mathscr{S}(v_{n-1}) - \mathscr{S}(\widetilde{v}_{n-1})$, we repeatedly apply Lemma 1 and 3 to obtain

$$\big\|\mathscr{S}(v_{n-1}) - \mathscr{S}(\widetilde{v}_{n-1})\big\|_{H^m} \leq \mathrm{e}^{|b_1|\, h\, C_3(m, V_{n1}, \widetilde{V}_{n1}) + |b_2|\, h\, C_3(m, V_{n2}, \widetilde{V}_{n2})}\, \|v_{n-1} - \widetilde{v}_{n-1}\|_{H^m}\,.$$

Clearly, for $d = 1$, $m \geq 1$, and $d = 2, 3$, $m \geq 2$, respectively, the quantities $C_3(m, V_{n1}, \widetilde{V}_{n1})$ and $C_3(m, V_{n2}, \widetilde{V}_{n2})$ are bounded, provided that v_{n-1} and $\widetilde{v}_{n-1}$ are bounded in $H^m(\mathbb{R}^d)$ and $\partial^\mu W \in L^\infty(\mathbb{R}^d)$ for $|\mu| \leq m$. For $d = 1$, $m = 0$, and $d = 2, 3$, $m = 0, 1$, respectively, we first derive the corresponding estimate in $H^j(\mathbb{R}^d)$ with integer $j \geq m$ given by (2.2b); then, the specified bound with respect to the norm in $H^m(\mathbb{R}^d)$ follows. □

6. Local error. In this section, we are concerned with deriving a suitable relation for the local error $d_n = \mathscr{E}(\widehat{u}_{n-1}) - \mathscr{S}(\widehat{u}_{n-1})$ of the exponential operator splitting method (3.2) under reasonable requirements on the exact solution of the nonlinear evolutionary Schrödinger equation (2.2); our approach is in the lines of [13, 14, 21]. In order to write the resulting relation for the local error in compact form, it is convenient to introduce several abbreviations.

6.1. Exact solution. Our main tool for expanding the exact solution value $\widehat{u}_n = \mathscr{E}(\widehat{u}_{n-1})$ is the variation-of-constants formula

$$\begin{aligned}
u(t_{n-1} + \tau_j) &= \mathrm{e}^{\tau_j A}\, \widehat{u}_{n-1}\\
&\quad + \int_0^{\tau_j} \mathrm{e}^{(\tau_j - \tau_{j+1}) A}\, B\big(u(t_{n-1} + \tau_{j+1})\big)\, u(t_{n-1} + \tau_{j+1})\, \mathrm{d}\tau_{j+1}\,.
\end{aligned} \tag{6.1}$$

More precisely, we repeatedly apply the above relation (6.1) to $\widehat{u}_n = u(t_{n-1}+h)$; step by step we obtain $\widehat{u}_n = \mathrm{e}^{hA}\,\widehat{u}_{n-1} + \widehat{R}_1 = \mathrm{e}^{hA}\,\widehat{u}_{n-1} + \widehat{I}_1 + \widehat{R}_2$ which finally yields

$$\widehat{u}_n = \mathrm{e}^{hA}\,\widehat{u}_{n-1} + \widehat{I}_1 + \widehat{I}_2 + \widehat{R}_3\,; \tag{6.2a}$$

here, we employ the following abbreviations

$$\begin{gathered}
\widehat{f}_1(\tau_1) = \mathrm{e}^{(h-\tau_1)A}\,B\big(u(t_{n-1}+\tau_1)\big)\,,\\
\widehat{f}_2(\tau_1,\tau_2) = \widehat{f}_1(\tau_1)\,\mathrm{e}^{(\tau_1-\tau_2)A}\,B\big(u(t_{n-1}+\tau_2)\big)\,,\\
\widehat{g}_1(\tau_1) = \widehat{f}_1(\tau_1)\,\mathrm{e}^{\tau_1 A}\,\widehat{u}_{n-1}\,, \quad \widehat{g}_2(\tau_1,\tau_2) = \widehat{f}_2(\tau_1,\tau_2)\,\mathrm{e}^{\tau_2 A}\,\widehat{u}_{n-1}\,,\\
\Delta_1 = [0,h], \quad \Delta_2 = \big\{\tau = (\tau_1,\tau_2)\in\mathbb{R}^2 : 0\le\tau_2\le\tau_1\le h\big\},\\
\Delta_3 = \big\{\tau = (\tau_1,\tau_2,\tau_3)\in\mathbb{R}^3 : 0\le\tau_3\le\tau_2\le\tau_1\le h\big\},\\
\widehat{I}_k = \int_{\Delta_k}\widehat{g}_k(\tau)\,\mathrm{d}\tau\,, \quad \widehat{R}_k = \int_{\Delta_k}\widehat{f}_k(\tau)\,u(t_{n-1}+\tau_j)\,\mathrm{d}\tau\,.
\end{gathered} \tag{6.2b}$$

Under the assumption that the exact solution is bounded in $H^j\big(\mathbb{R}^d\big)$ and that the potential satisfies $\partial^\mu W \in L^\infty\big(\mathbb{R}^d\big)$ for $|\mu|\le j$ with j given by (2.2b), the remainder $\widehat{R}_3$ fulfills the bound

$$\big\|\widehat{R}_3\big\|_{H^m} \le C\,h^3\,,$$

see Lemma 1-3; in particular, C depends on the quantities $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu|\le j\big\}$, $\max\big\{\|u(t)\|_{H^j} : t_{n-1}\le t\le t_n\big\}$, and on ϑ.

6.2. Numerical approximation. An expansion of the numerical approximation $\mathscr{S}(\widehat{u}_{n-1})$ that resembles (6.2) is obtained by means of the recurrence relation (1.4) for the φ-functions and the algebraic identity

$$\prod_{j=1}^{J}\big(K_j + L_j\big) = \prod_{\ell=1}^{J} K_\ell + \sum_{j=1}^{J}\prod_{\ell=j+1}^{J} K_\ell\, L_j \prod_{\ell=1}^{j-1}\big(K_\ell + L_\ell\big) \tag{6.3}$$

that is valid for operators $K_j, L_j : H^m\big(\mathbb{R}^d\big)\to H^m\big(\mathbb{R}^d\big)$, $1\le j\le J$. In order to make use of a recursive procedure, we further introduce the nonlinear operators

$$\begin{gathered}
\mathscr{S}_j(\widehat{u}_{n-1}) = \prod_{\ell=1}^{j}\mathrm{e}^{\,b_\ell hB(\widehat{U}_{n\ell})}\,\mathrm{e}^{a_\ell hA}\;\widehat{u}_{n-1}\,, \quad j=1,2\,, \qquad \mathscr{S}_0 = I\,,\\
\widehat{U}_{n1} = \mathrm{e}^{a_1 hA}\,\widehat{u}_{n-1}\,, \qquad \widehat{U}_{n2} = \mathrm{e}^{a_2 hA}\;\mathrm{e}^{\,b_1 hB(\widehat{U}_{n1})}\,\widehat{U}_{n1}\,;
\end{gathered} \tag{6.4}$$

clearly, it holds $\mathscr{S}(\widehat{u}_{n-1}) = \mathscr{S}_2(\widehat{u}_{n-1})$. In a first step, by means of the identity $\mathrm{e}^{b_j hB(\widehat{U}_{nj})} = I + b_j hB(\widehat{U}_{nj})\,\varphi_1\big(b_j hB(\widehat{U}_{nj})\big)$ and (6.3), we obtain

$$\begin{aligned}
\mathscr{S}(\widehat{u}_{n-1}) &= \prod_{j=1}^{2}\Big(\mathrm{e}^{a_j hA} + b_j hB(\widehat{U}_{nj})\,\varphi_1\big(b_j hB(\widehat{U}_{nj})\big)\,\mathrm{e}^{a_j hA}\Big)\;\widehat{u}_{n-1}\\
&= \mathrm{e}^{hA}\;\widehat{u}_{n-1}\\
&\qquad + h\sum_{j=1}^{2} b_j\,\mathrm{e}^{(1-c_j)\,hA}\;B(\widehat{U}_{nj})\,\varphi_1\big(b_j hB(\widehat{U}_{nj})\big)\,\mathrm{e}^{a_j hA}\,\mathscr{S}_{j-1}(\widehat{u}_{n-1})\,,
\end{aligned} \tag{6.5}$$

where $c_1 = a_1$ and $c_2 = a_1 + a_2 = 1$, see (3.2b). We next replace $\mathscr{S}_1(\widehat{u}_{n-1})$ by the analogue of (6.5)

$$\mathrm{e}^{a_2 hA} \mathscr{S}_1(\widehat{u}_{n-1}) = \mathrm{e}^{hA}\,\widehat{u}_{n-1} + h\,b_1\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})\,\varphi_1\big(b_1 hB(\widehat{U}_{n1})\big)\,\mathrm{e}^{a_1 hA}\,\widehat{u}_{n-1}$$

and apply (1.4); this finally yields the expansion

$$\mathscr{S}(\widehat{u}_{n-1}) = \mathrm{e}^{hA}\,\widehat{u}_{n-1} + Q_1 + Q_2 + R_3 \tag{6.6a}$$

which involves the following sums

$$\begin{aligned} Q_1 &= h\Big(b_1\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})\,\mathrm{e}^{a_1 hA} + b_2\,B(\widehat{U}_{n2})\,\mathrm{e}^{hA}\Big)\,\widehat{u}_{n-1}\,, \\ Q_2 &= \tfrac{1}{2}\,h^2\Big(b_1^2\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})^2\,\mathrm{e}^{a_1 hA} + 2\,b_1 b_2\,B(\widehat{U}_{n2})\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})\,\mathrm{e}^{a_1 hA} \\ &\qquad + b_2^2\,B(\widehat{U}_{n2})^2\,\mathrm{e}^{hA}\Big)\,\widehat{u}_{n-1}\,, \end{aligned} \tag{6.6b}$$

and further the remainder

$$\begin{aligned} R_3 = h^3\Big(&b_1^3\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})^3\varphi_3\big(b_1 hB(\widehat{U}_{n1})\big)\,\mathrm{e}^{a_1 hA} \\ &+ b_1^2 b_2\,B(\widehat{U}_{n2})\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})^2\,\varphi_2\big(b_1 hB(\widehat{U}_{n1})\big)\,\mathrm{e}^{a_1 hA} \\ &\quad + b_1 b_2^2\,B(\widehat{U}_{n2})^2\,\varphi_2\big(b_2 hB(\widehat{U}_{n2})\big)\,\mathrm{e}^{a_2 hA}\,B(\widehat{U}_{n1})\,\varphi_1\big(b_1 hB(\widehat{U}_{n1})\big) \\ &\qquad \times\,\mathrm{e}^{a_1 hA} + b_2^3\,B(\widehat{U}_{n2})^3\,\varphi_3\big(b_2 hB(\widehat{U}_{n2})\big)\,\mathrm{e}^{hA}\Big)\,\widehat{u}_{n-1}\,. \end{aligned} \tag{6.6c}$$

Similarly to before, by Lemma 1-3 and relation (B.4), we obtain the bound

$$\big\|R_3\big\|_{H^m} \le C\,h^3$$

with a constant C depending on $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \le j\big\}$, ϑ, and further on $\max\big\{\|u(t)\|_{H^j} : t_{n-1} \le t \le t_n\big\}$.

6.3. Local error expansion. The above expansions (6.2) and (6.6) imply the following relation for the local error

$$d_n = \mathscr{E}(\widehat{u}_{n-1}) - \mathscr{S}(\widehat{u}_{n-1}) = \sum_{k=1}^{2}(\widehat{I}_k - Q_k) + \widehat{R}_3 - R_3\,. \tag{6.7a}$$

In order to expand the local error d_n further, we make use of the fact that the sum Q_k is related to a quadrature formula approximation of the integral $\widehat{I}_k$; more precisely, we rewrite (6.7a) as follows

$$d_n = \widehat{S}_3 + S_3 + \widehat{R}_3 - R_3\,, \qquad \widehat{S}_3 = \sum_{k=1}^{2}\big(\widehat{I}_k - \widehat{Q}_k\big)\,, \quad S_3 = \sum_{k=1}^{2}\big(\widehat{Q}_k - Q_k\big)\,, \tag{6.7b}$$

where $\widehat{Q}_1$ and $\widehat{Q}_2$ are defined through

$$\begin{aligned} \widehat{Q}_1 &= h\,\Big(b_1\,\mathrm{e}^{a_2 hA}\,B\big(u(t_{n-1}+a_1 h)\big)\,\mathrm{e}^{a_1 hA} + b_2\,B\big(u(t_n)\big)\,\mathrm{e}^{hA}\Big)\,\widehat{u}_{n-1}\,, \\ \widehat{Q}_2 &= \tfrac{1}{2}\,h^2\,\Big(b_1^2\,\mathrm{e}^{a_2 hA}\,B\big(u(t_{n-1}+a_1 h)\big)^2\,\mathrm{e}^{a_1 hA} \\ &\qquad + 2\,b_1 b_2\,B\big(u(t_n)\big)\,\mathrm{e}^{a_2 hA}\,B\big(u(t_{n-1}+a_1 h)\big)\,\mathrm{e}^{a_1 hA} \\ &\qquad\quad + b_2^2\,B\big(u(t_n)\big)^2\,\mathrm{e}^{hA}\Big)\,\widehat{u}_{n-1}\,. \end{aligned} \tag{6.7c}$$

With the help of the abbreviations introduced in (6.2) and additional coefficients $\alpha_{11} = \alpha_{22} = 1$ and $\alpha_{21} = 2$, the first sum $\widehat{S}_3$ in (6.7b) takes the compact form

$$\widehat{S}_3 = \int_0^h \Big(\widehat{g}_1(\tau_1) - \sum_{\lambda_1=1}^{2} b_{\lambda_1}\, \widehat{g}_1(c_{\lambda_1} h)\Big)\, \mathrm{d}\tau_1 \\ + \int_0^h \int_0^{\tau_1} \Big(\widehat{g}_2(\tau_1,\tau_2) - \sum_{\lambda_1=1}^{2} \sum_{\lambda_2=1}^{\lambda_1} \alpha_{\lambda_1\lambda_2}\, b_{\lambda_1} b_{\lambda_2}\, \widehat{g}_2(c_{\lambda_1} h, c_{\lambda_2} h)\Big)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,.$$

Employing Taylor series expansions of $\widehat{g}_1$ and $\widehat{g}_2$ about zero and applying the order conditions (3.2b), we obtain

$$\begin{aligned} \widehat{S}_3 = {} & \int_0^h \int_0^1 (1-\sigma) \Big(\tau_1^2\, \partial_{\tau_1}^2 \widehat{g}_1(\sigma\tau_1) - h^2 \sum_{\lambda_1=1}^{2} b_{\lambda_1} c_{\lambda_1}^2\, \partial_{\tau_1}^2 \widehat{g}_1(\sigma c_{\lambda_1} h)\Big)\, \mathrm{d}\sigma\, \mathrm{d}\tau_1 \\ & + \int_0^h \int_0^{\tau_1} \int_0^1 \Big(\tau_1 \partial_{\tau_1} \widehat{g}_2(\sigma\tau_1,\sigma\tau_2) + \tau_2\, \partial_{\tau_2} \widehat{g}_2(\sigma\tau_1,\sigma\tau_2) \\ & \qquad - h \sum_{\lambda_1=1}^{2} \sum_{\lambda_2=1}^{\lambda_1} \alpha_{\lambda_1\lambda_2}\, b_{\lambda_1} b_{\lambda_2} \Big(c_{\lambda_1} \partial_{\tau_1} \widehat{g}_2(\sigma c_{\lambda_1} h, \sigma c_{\lambda_2} h) \\ & \qquad\qquad + c_{\lambda_2} \partial_{\tau_2} \widehat{g}_2(\sigma\, c_{\lambda_1} h, \sigma c_{\lambda_2} h)\Big)\Big)\, \mathrm{d}\sigma\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,; \end{aligned} \tag{6.7d}$$

the derivatives of $\widehat{g}_j(\tau)$ are determined in Section B.4. Regarding the second sum S_3 in (6.7b), it is seen that $\widehat{Q}_k$ and Q_k only differ in the arguments of B. More precisely, $\widehat{Q}_k - Q_k$ can be rewritten in such a way that each term involves a difference $G_j(h)$ where

$$G_j(\tau) = B\big(u(t_{n-1} + c_j\, \tau)\big) - B\big(\widehat{U}_{nj}(\tau)\big)\,, \qquad j = 1, 2\,; \tag{6.7e}$$

here, we consider $\widehat{U}_{n1}(\tau) = \mathrm{e}^{a_1 \tau A}\, \widehat{u}_{n-1}$ and $\widehat{U}_{n2}(\tau) = \mathrm{e}^{a_2 \tau A}\ \mathrm{e}^{b_1 \tau B(\widehat{U}_{n1}(\tau))}\, \widehat{U}_{n1}(\tau)$ as functions of τ, see also (6.4). We thus have

$$\begin{aligned} S_3 = h\, & \Big(b_1\, \mathrm{e}^{a_2 h A}\, G_1(h)\, \mathrm{e}^{a_1 h A} + b_2\, G_2(h)\, \mathrm{e}^{hA}\Big)\, \widehat{u}_{n-1}\,, \\ & + \tfrac{1}{2}\, h^2 \Big(b_1^2\, \mathrm{e}^{a_2 h A} \Big(B\big(u(t_{n-1} + a_1 h)\big) + B\big(\widehat{U}_{n1}(h)\big)\Big)\, G_1(h)\, \mathrm{e}^{a_1 h A} \\ & \qquad + 2\, b_1 b_2 \Big(G_2(h)\, \mathrm{e}^{a_2 h A}\, B\big(u(t_{n-1} + a_1 h)\big) + B\big(\widehat{U}_{n2}(h)\big)\, \mathrm{e}^{a_2 h A}\, G_1(h)\Big)\, \mathrm{e}^{a_1 h A} \\ & \qquad\quad + b_2^2 \Big(B\big(u(t_n)\big) + B\big(\widehat{U}_{n2}(h)\big)\Big)\, G_2(h)\, \mathrm{e}^{hA}\Big)\, \widehat{u}_{n-1}\,. \end{aligned}$$

We next employ a Taylor series expansion of G_j about zero up to order $3-k$; the required derivatives of G_j are given in Section B.4. Clearly, it holds $\widehat{U}_{nj}(0) = \widehat{u}_{n-1}$ and thus $G_j(0) = 0$ for $j = 1, 2$. Due to the fact that $\partial_\tau \widehat{U}_{n1}(0) = a_1 A\, \widehat{u}_{n-1}$ and $\partial_\tau \widehat{U}_{n2}(0) = A\, \widehat{u}_{n-1} + a_1 b_1 B'(\widehat{u}_{n-1})\big(A\, \widehat{u}_{n-1}\big)\, \widehat{u}_{n-1}$, we further obtain

$$\begin{aligned} \partial_\tau G_1(0) &= a_1\, B'(\widehat{u}_{n-1})\, B(\widehat{u}_{n-1})\, \widehat{u}_{n-1}\,, \\ \partial_\tau G_2(0) &= B'(\widehat{u}_{n-1})\, \big(B(\widehat{u}_{n-1})\, \widehat{u}_{n-1} - a_1 b_1 B'(\widehat{u}_{n-1})\big(A\, \widehat{u}_{n-1}\big)\, \widehat{u}_{n-1}\big)\,, \end{aligned}$$

see also (3.2b) and (B.6). Using that $B(\widehat{u}_{n-1})$ as well as

$$\big(B'(\widehat{u}_{n-1})\big)(A\,\widehat{u}_{n-1}) = -\,2\,\mathrm{i}\,\vartheta\,\Re\big(\overline{\widehat{u}_{n-1}}\,(A\,\widehat{u}_{n-1})\big)$$

are purely imaginary, it follows that $G_j'(0) = 0$ for $j = 1, 2$, see (B.5a). From a Taylor series expansion of $G_j(h)$ about zero we thus have

$$G_j(h) = h\int_0^1 \partial_\tau G_j(\sigma\,h)\,\mathrm{d}\sigma = h^2\int_0^1 (1-\sigma)\,\partial_\tau^2\,G_j(\sigma h)\,\mathrm{d}\sigma\,;$$

this finally yields the identity

$$\begin{aligned}
S_3 = h^3 \int_0^1 \Bigg(&(1-\sigma)\,\Big(b_1\,\mathrm{e}^{a_2 hA}\,\partial_\tau^2\,G_1(\sigma h)\,\mathrm{e}^{a_1 hA} + b_2\,\partial_\tau^2\,G_1(\sigma h)\,\mathrm{e}^{hA}\Big)\\
&+ \tfrac{1}{2}\,b_1^2\,\mathrm{e}^{a_2 hA}\,\Big(B\big(u(t_{n-1}+a_1 h)\big) + B\big(\widehat{U}_{n1}(h)\big)\Big)\,\partial_\tau G_1(\sigma\,h)\,\mathrm{e}^{a_1 hA}\\
&+ b_1 b_2\Big(\partial_\tau G_2(\sigma\,h)\,\mathrm{e}^{a_2 hA}\,B\big(u(t_{n-1}+a_1 h)\big)\\
&+ B\big(\widehat{U}_{n2}(h)\big)\,\mathrm{e}^{a_2 hA}\,\partial_\tau G_1(\sigma\,h)\Big)\,\mathrm{e}^{a_1 hA}\\
&+ \tfrac{1}{2} b_2^2\,\Big(B\big(u(t_n)\big) + B\big(\widehat{U}_{n2}(h)\big)\Big)\,\partial_\tau G_2(\sigma\,h)\,\mathrm{e}^{hA}\Bigg)\,\widehat{u}_{n-1}\,\mathrm{d}\sigma\,.
\end{aligned} \tag{6.7f}$$

Provided that the exact solution u and the potential W fulfill suitable regularity requirements, the derivatives $\partial_{\tau_1}^2\widehat{g}_1$, $\partial_{\tau_j}\widehat{g}_2$, $\partial_\tau G_j$, and $\partial_\tau^2\,G_1$ are bounded in $H^m\big(\mathbb{R}^d\big)$; more precisely, we suppose that the exact solution of (2.2) fulfills the assumption $u(t) \in D_{j,4}\big(\mathbb{R}^d\big)$ for $t_{n-1} \le t \le t_n$, see (1.3) and (2.2b) for the definition of $D_{j,4}\big(\mathbb{R}^d\big)$. Altogether, we obtain the following estimate for the local error

$$\big\|d_n\big\|_{H^m} \le C\,h^3\,, \tag{6.8}$$

see (6.7b), (6.7d), and (6.7f); here, we require $\max\big\{\|\partial^\mu W\|_{L^\infty} : |\mu| \le j+4\big\}$ and $\max\big\{\|u(t)\|_{D_{j,4}} : t_{n-1} \le t \le t_n\big\}$ to be bounded.

Appendix A. Hermite functions. We let $H_{\mu_j} : \mathbb{R} \to \mathbb{R}$ denote the univariate Hermite polynomial of degree μ_j, normalised with respect to the weight function $w(\xi_j) = \mathrm{e}^{-\,\xi_j^2}$; that is, H_{μ_j} is defined through the recurrence relation

$$\begin{aligned}
H_0(\xi_j) &= \tfrac{1}{\sqrt[4]{\pi}}\,, \qquad H_1(\xi_j) = \sqrt{2}\,\xi_j\,H_0(\xi_j)\,,\\
H_{\mu_j}(\xi_j) &= \tfrac{1}{\sqrt{\mu_j}}\,\big(\sqrt{2}\,\xi_j\,H_{\mu_j-1}(\xi_j) - \sqrt{\mu_j-1}\,H_{\mu_j-2}(\xi_j)\big), \qquad \mu_j \ge 2\,.
\end{aligned} \tag{A.1}$$

The scaled and normalised Hermite functions $\mathscr{H}_\mu : \mathbb{R}^d \to \mathbb{R}$ are then given by

$$\mathscr{H}_\mu(\xi) = \prod_{j=1}^d \mathscr{H}_{\mu_j}(\xi_j)\,, \qquad \mathscr{H}_{\mu_j}(\xi_j) = H_{\mu_j}(\xi_j)\,\mathrm{e}^{-\,\frac{1}{2}\xi_j^2}\,.$$

As well known, the Hermite functions $(\mathscr{H}_\mu)$ form an orthonormal basis of the function space $L^2\big(\mathbb{R}^d\big)$; thus, for any $v \in L^2\big(\mathbb{R}^d\big)$ the representation

$$v = \sum_\mu v_\mu\,\mathscr{H}_\mu\,, \qquad v_\mu = \big(v \,\big|\, \mathscr{H}_\mu\big)_{L^2}\,, \tag{A.2a}$$

follows. Due to fact that the eigenvalue relation

$$\tfrac{1}{2}\big(-\Delta_\gamma + V_\gamma\big)\,\mathscr{H}_\mu = \lambda_\mu\,\mathscr{H}_\mu\,, \qquad \lambda_\mu = \sum_{j=1}^{d} \gamma_j\,\big(\mu_j + \tfrac{1}{2}\big)\,, \tag{A.2b}$$

holds, we further obtain

$$A\,v = -\,\mathrm{i}\sum_\mu v_\mu\,\lambda_\mu\,\mathscr{H}_\mu\,, \qquad \mathrm{e}^{tA}\,v = \sum_\mu v_\mu\,\mathrm{e}^{-\,\mathrm{i}\,t\,\lambda_\mu}\,\mathscr{H}_\mu\,, \tag{A.2c}$$

see (2.2). We finally note that relation (A.1) implies

$$\begin{gathered}\partial_{\xi_j}\mathscr{H}_0 = 0\,, \qquad \partial_{\xi_j}\mathscr{H}_1 = -\,\mathscr{H}_2\,,\\ \partial_{\xi_j}\mathscr{H}_{\mu_j} = -\,\tfrac{1}{\sqrt{2}}\,\big(\sqrt{\mu_j+1}\,\mathscr{H}_{\mu_j+1} - \sqrt{\mu_j}\,\mathscr{H}_{\mu_j-1}\big), \quad \mu_j \geq 2\,;\end{gathered}$$

as a consequence, any partial derivative $\partial^\kappa \mathscr{H}_\mu$ can be expressed as a (finite) linear combination of the form

$$\partial^\kappa \mathscr{H}_\mu = \sum_\nu c_\nu\,\mathscr{H}_\nu \tag{A.3}$$

involving certain coefficients $c_\nu \in \mathbb{R}$.

Appendix B. Gross–Pitaevskii equation. In this appendix, we collect several auxiliary results that are applied in Section 4 for the derivation of Theorem 1 and 2. In Section B.1, we indicate how to transform the GPE (1.1) to the normalised equation (2.1). Then, we are concerned with conserved quantities of the GPE (2.1), see Section B.2. Section B.3 is finally devoted to auxiliary estimates involving the operators A and B, see also (2.2).

B.1. Normalisation. We consider the original formulation (1.1) of the GPE

$$\begin{gathered}\mathrm{i}\,\hbar\,\partial_t\Psi(x,t) = \Big(-\,\tfrac{\hbar^2}{2\,m}\,\Delta + U(x) + \tfrac{4\pi\hbar^2 aN}{m}\,\big|\Psi(x,t)\big|^2\Big)\,\Psi(x,t)\,, \qquad x\in\mathbb{R}^d\,, \quad t\geq 0\,,\\ \Delta = \sum_{j=1}^{d}\partial_{x_j}^2\,, \qquad U(x) = \tfrac{m}{2}\sum_{j=1}^{d}(\gamma_j\,x_j)^2 + U_0(x)\,;\end{gathered}$$

here, we suppose U to be a quasi-harmonic potential involving positive coefficients γ_j, $1 \leq j \leq d$. We apply the linear transformation $\xi_j = \sqrt{c_j}\,x_j$ with $c_j = \frac{m\,\gamma_j}{\hbar}$ for $1 \leq j \leq d$; using that $\partial_{x_j}^2 = c_j\,\partial_{\xi_j}^2$ and setting

$$\psi(\xi,t) = \frac{1}{\sqrt[4]{c_1\cdots c_d}}\,\Psi(x,t)$$

as well as $W(\xi) = \frac{1}{\hbar}\,U_0(x)$, and $\vartheta = \frac{4\pi\hbar aN}{m}\sqrt{c_1\cdots c_d}$, we thus obtain

$$\begin{gathered}\mathrm{i}\,\partial_t\psi(\xi,t) = \Big(-\,\tfrac{1}{2}\,\Delta_\gamma + V(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2\Big)\,\psi(\xi,t)\,, \qquad \xi\in\mathbb{R}^d\,, \quad t\geq 0\,,\\ \Delta_\gamma = \sum_{j=1}^{d}\gamma_j\,\partial_{\xi_j}^2\,, \qquad V(\xi) = \tfrac{1}{2}\,V_\gamma(\xi) + W(\xi)\,, \qquad V_\gamma(\xi) = \sum_{j=1}^{d}\gamma_j\,\xi_j^2\,,\end{gathered}$$

see (2.1). We further note that $\|\psi(\cdot,t)\|_{L^2} = \|\Psi(\cdot,t)\|_{L^2}$.

B.2. Conserved quantities. For notational brevity, we meanwhile omit t and write $\psi(\xi) = \psi(\xi, t)$ for short.

Particle number conservation. For proving the preservation of the particle number $\|\psi\|_{L^2}^2$, we employ a partial integration

$$\big(\partial_{\xi_j}^2 \, \psi \,|\, \psi\big)_{L^2} = -\int_{\mathbb{R}^d} \partial_{\xi_j} \psi(\xi) \, \partial_{\xi_j} \overline{\psi(\xi)} \, \mathrm{d}\xi = -\, \|\partial_{\xi_j} \psi\|_{L^2}$$

and conclude $(\Delta_\gamma \, \psi \,|\, \psi)_{L^2} \in \mathbb{R}$. Consequently, by means of the GPE (2.1), we obtain

$$(\partial_t \psi \,|\, \psi)_{L^2} = -\,\mathrm{i} \Big(-\tfrac{1}{2} \, (\Delta_\gamma \, \psi \,|\, \psi)_{L^2} + (V \, \psi \,|\, \psi)_{L^2} + \vartheta \, \big(|\psi|^2 \, \psi \,|\, \psi\big)_{L^2} \Big) \in \mathrm{i} \, \mathbb{R} \, ,$$

and thus the desired result $\partial_t \|\psi\|_{L^2}^2 = \partial_t (\psi \,|\, \psi)_{L^2} = 2 \, \Re (\partial_t \psi \,|\, \psi)_{L^2} = 0$ follows.

Energy conservation. In order to show that the energy functional (2.3) is time-independent, we consider its time derivative

$$\partial_t E(\psi) = 2 \, \Re \Big(\big(-\tfrac{1}{2} \, \Delta_\gamma + V + \vartheta \, |\psi|^2 \big) \psi \, \Big| \, \partial_t \psi \Big)_{L^2} ;$$

regarding (2.1) and making use of the fact that

$$\mathrm{i} \, \|\partial_t \psi\|_{L^2} = \mathrm{i} \, (\partial_t \psi \,|\, \partial_t \psi)_{L^2} = \Big(\big(-\tfrac{1}{2} \, \Delta_\gamma + V + \vartheta \, |\psi|^2 \big) \psi \, \Big| \, \partial_t \psi \Big)_{L^2} \in \mathrm{i} \, \mathbb{R} \, ,$$

it follows $\partial_t E(\psi) = 0$.

Invariance. The time-invariance of $|\psi|$ with ψ being the solution of the differential equation $\partial_t \psi = -\,\mathrm{i} \, \big(W \psi + \vartheta \, |\psi|^2 \, \psi \big)$, see (2.2) and (3.1), follows in a straightforward way from the fact that $\overline{\psi} \, \partial_t \psi = -\,\mathrm{i} \, \big(W |\psi|^2 + \vartheta \, |\psi|^4 \big) \in \mathrm{i} \, \mathbb{R}$, wherefore we obtain $\partial_t |\psi|^2 = 2 \, \Re \big(\overline{\psi} \, \partial_t \psi \big) = 0$.

B.3. Auxiliary estimates. In the following, we derive estimates for the solutions of (3.1); for the definition of A and B, we refer to (2.2). Basic results on Hermite functions that are useful for a proof of Lemma 1 are reviewed in Appendix A.

LEMMA 1. For any integer $m \geq 0$ it holds

$$\big\| \mathrm{e}^{tA} \big\|_{H^m \leftarrow H^m} = 1 \, , \qquad t \geq 0 \, ;$$

that is, the linear operator e^{tA} is unitary on $H^m\big(\mathbb{R}^d\big)$.

Proof. In order to prove the statement of Lemma 1, it suffices to show the relation

$$\big\| \partial^\kappa \, \mathrm{e}^{tA} \, v \big\|_{L^2} = \big\| \partial^\kappa \, v \big\|_{L^2} \, , \qquad |\kappa| \leq m \, , \quad t \geq 0 \, , \quad v \in H^m\big(\mathbb{R}^d\big) \, .$$

Employing a spectral decomposition into Hermite basis functions, we have

$$v = \sum_\mu v_\mu \, \mathscr{H}_\mu \, , \qquad \mathrm{e}^{tA} \, v = \sum_\mu v_\mu \, \mathrm{e}^{-\,\mathrm{i}\, t \, \lambda_\mu} \, \mathscr{H}_\mu \, ,$$

see also (A.2); further, by means of (A.3), we obtain

$$\partial^\kappa \, v = \sum_\mu v_\mu \, \partial^\kappa \mathscr{H}_\mu = \sum_\mu \widetilde{v}_\mu \, \mathscr{H}_\mu \, , \qquad \partial^\kappa \, \mathrm{e}^{tA} \, v = \sum_\mu \widetilde{v}_\mu \, \mathrm{e}^{-\,\mathrm{i}\, t \, \lambda_\mu} \, \mathscr{H}_\mu,$$

with certain coefficients $\widetilde{v}_\mu$. Making use of the fact that $\big| \mathrm{e}^{-\,\mathrm{i}\, t \, \lambda_\mu} \big| = 1$ and that the orthonormality relation $\big(\mathscr{H}_\kappa \, \big| \, \mathscr{H}_\mu \big)_{L^2} = \delta_{\kappa\mu}$ is valid, it follows

$$\big\| \partial^\kappa \, \mathrm{e}^{tA} \, v \big\|_{L^2}^2 = \sum_\mu |\widetilde{v}_\mu|^2 = \big\| \partial^\kappa \, v \big\|_{L^2}^2 \, , \qquad |\kappa| \leq m \, , \quad t \geq 0 \, , \quad v \in H^m\big(\mathbb{R}^d\big) \, ,$$

which yields the desired result. ◻

For the convenience of the reader, we recapitulate the continuous embeddings

$$\begin{cases} H^{j+m}\big(\mathbb{R}^d\big) \subset \mathscr{C}_B^j\big(\mathbb{R}^d\big) & \text{if } d=1\,,\ m \geq 1\,, \\ H^{j+1}\big(\mathbb{R}^d\big) \subset W^{j,q}\big(\mathbb{R}^d\big) & \text{if } d=2\,,\ 2 \leq q < \infty\,, \\ H^{j+m}\big(\mathbb{R}^d\big) \subset \mathscr{C}_B^j\big(\mathbb{R}^d\big) & \text{if } d=2\,,\ m > 1\,, \\ H^{j+m}\big(\mathbb{R}^d\big) \subset W^{j,q}\big(\mathbb{R}^d\big) & \text{if } d=3\,,\ 2 \leq q \leq \frac{2d}{d-2m}\,,\ m < \frac{1}{2}\,d\,, \\ H^{j+m}\big(\mathbb{R}^d\big) \subset W^{j,q}\big(\mathbb{R}^d\big) & \text{if } d=3\,,\ 2 \leq q < \infty\,,\ m = \frac{1}{2}\,d\,, \\ H^{j+m}\big(\mathbb{R}^d\big) \subset \mathscr{C}_B^j\big(\mathbb{R}^d\big) & \text{if } d=3\,,\ m > \frac{1}{2}\,d\,; \end{cases} \tag{B.1}$$

see Adams [1]. These relations are needed for the derivation of Lemma 2; more precisely, in the proof of Lemma 2 we apply the estimate

$$\|u\,v\,w\|_{H^m} \leq C\,\|u\|_{H^j}\,\|v\|_{H^j}\,\|w\|_{H^m}\,, \tag{B.2}$$

where j is given by (2.2b). The above bound follows from Hölder's inequality

$$\|u\,v\,w\|_{L^2} \leq C\,\|u\|_{L^{2p}(\mathbb{R}^d)}\,\|v\|_{L^{2q}(\mathbb{R}^d)}\,\|w\|_{L^{2r}(\mathbb{R}^d)}, \qquad \tfrac{1}{p}+\tfrac{1}{q}+\tfrac{1}{r}=1\,,$$

with $p=q=\infty, r=1$ and $p=q=r=3$, respectively, together with (B.1). Namely, for $d=1$, due to $H^1\big(\mathbb{R}^d\big) \subset L^\infty\big(\mathbb{R}^d\big)$, we obtain

$$\|u\,v\,w\|_{L^2} \leq C\,\|u\|_{H^1}\,\|v\|_{H^1}\,\|w\|_{L^2}\,; \tag{B.3a}$$

differentiation and a repeated application of (B.3a) further yields

$$\|u\,v\,w\|_{H^m} \leq C\,\|u\|_{H^m}\,\|v\|_{H^m}\,\|w\|_{H^m}\,, \qquad m \geq 1\,. \tag{B.3b}$$

On the other hand, for $d=2,3$, the continuous embeddings $H^1\big(\mathbb{R}^d\big) \subset L^6\big(\mathbb{R}^d\big)$ and $H^2\big(\mathbb{R}^d\big) \subset L^\infty\big(\mathbb{R}^d\big)$ imply the bounds

$$\|u\,v\,w\|_{L^2} \leq C\,\|u\|_{H^1}\,\|v\|_{H^1}\,\|w\|_{H^1}\,, \qquad \|u\,v\,w\|_{L^2} \leq C\,\|u\|_{H^2}\,\|v\|_{H^2}\,\|w\|_{L^2}\,; \tag{B.3c}$$

as a consequence, we obtain

$$\begin{aligned} \|u\,v\,w\|_{H^1} &\leq C\,\|u\|_{H^2}\,\|v\|_{H^2}\,\|w\|_{H^1}\,, \\ \|u\,v\,w\|_{H^m} &\leq C\,\|u\|_{H^m}\,\|v\|_{H^m}\,\|w\|_{H^m}\,, \qquad m \geq 2\,. \end{aligned} \tag{B.3d}$$

Altogether, this yields (B.2).

Lemma 2. For some $m \geq 0$ let j be defined through (2.2b). Then, the estimates

$$\begin{aligned} \big\|B(v)\big\|_{H^m \leftarrow H^m} &\leq C_1(m,v)\,, \\ \big\|B(v)-B(w)\big\|_{H^m \leftarrow H^j} &\leq C_2(m,v,w)\,\|v-w\|_{H^m}\,, \end{aligned}$$

are valid with $C_1(m,v)$ and $C_2(m,v,w)$ given by

$$\begin{aligned} C_1(m,v) &= C\,\Big(\max_{|\mu|\leq m}\big\|\partial^\mu W\big\|_{L^\infty} + \vartheta\,\|v\|_{H^j}^2\Big)\,, \\ C_2(m,v,w) &= C\,\vartheta\,\big(\|v\|_{H^j}+\|w\|_{H^j}\big)\,. \end{aligned}$$

Proof. (i) Let $v \in H^m(\mathbb{R}^d)$. The definition of the Sobolev norm (1.2) implies $\|Wv\|_{H^m} \le C \max\big\{\|\partial^\mu W\|_{L^\infty(\mathbb{R}^d)}\,\|v\|_{H^m} : |\mu| \le m\big\}$ and therefore

$$\big\|W\big\|_{H^m \leftarrow H^m} \le C \max_{|\mu|\le m} \big\|\partial^\mu W\big\|_{L^\infty(\mathbb{R}^d)}\,.$$

In order to estimate the operator norm of $\vartheta\,\overline{v}\,v : H^m(\mathbb{R}^d) \to H^m(\mathbb{R}^d)$, we apply (B.2); altogether this yields the given bound.

(ii) The statement concerning

$$B(v) - B(w) = -\,\mathrm{i}\,\vartheta\,\big(v\,\overline{v} - w\,\overline{w}\big) = -\,\mathrm{i}\,\vartheta\,\big(\overline{v}\,(v-w) + w\,\overline{(v-w)}\big)$$

follows in a similar manner by means of (B.2). ☐

Lemma 2 implies that $\varphi_k\big(tB(v)\big)$ is a bounded operator on $H^m(\mathbb{R}^d)$, see (1.4) for the definition of φ; more precisely, we have

$$\big\|\varphi_k\big(tB(v)\big)\big\|_{H^m \leftarrow H^m} \le \tfrac{1}{k!}\,\mathrm{e}^{C_1(m,v)\,t}\,, \qquad t \ge 0, \quad k \ge 0\,. \tag{B.4a}$$

Especially, for $k = 0$ and $m = 0$ the improved bound

$$\big\|\mathrm{e}^{tB(v)}\big\|_{L^2 \leftarrow L^2} = 1\,, \qquad t \ge 0\,, \tag{B.4b}$$

is valid; making use of the fact that $B(v)(\xi) \in \mathrm{i}\mathbb{R}$ for all $\xi \in \mathbb{R}^d$, the above relation follows from the identity

$$\big\|\mathrm{e}^{tB(v)}\,w\big\|_{L^2}^2 = \int_{\mathbb{R}^d} \big|\mathrm{e}^{tB(v)(\xi)}\big|^2\,\big|w(\xi)\big|^2\,\mathrm{d}\xi = \int_{\mathbb{R}^d} \big|w(\xi)\big|^2\,\mathrm{d}\xi = \|w\|_{L^2}^2\,.$$

The following lemma is essential in view of our stability result; the quantities C_1 and C_2 were introduced in Lemma 2.

Lemma 3. The following estimate

$$\big\|\mathrm{e}^{tB(v_0)}\,v_0 - \mathrm{e}^{tB(\widetilde{v}_0)}\,\widetilde{v}_0\big\|_{H^m} \le \mathrm{e}^{t\,C_3(m,v_0,\widetilde{v}_0)}\,\|v_0 - \widetilde{v}_0\|_{H^m}\,, \qquad t \ge 0, \quad m \ge 0\,,$$

is valid with constant given by

$$\begin{aligned} C_3(m,v_0,\widetilde{v}_0) &= \varphi_1\big(t\,C_1(j,\widetilde{v}_0)\big)\,C_2(m,v_0,\widetilde{v}_0)\,\|\widetilde{v}_0\|_{H^j}\,, \qquad m = 0\,,\\ C_3(m,v_0,\widetilde{v}_0) &= C_1(m,v_0) + \varphi_1\big(t\,C_1(j,\widetilde{v}_0)\big)\,C_2(m,v_0,\widetilde{v}_0)\,\|\widetilde{v}_0\|_{H^j}\,, \qquad m > 0\,; \end{aligned}$$

here, the integer $j \ge m$ is defined through (2.2b).

Proof. In order to prove Lemma 3, we relate $v(t) = \mathrm{e}^{tB(v_0)}\,v_0$ and $\widetilde{v}(t) = \mathrm{e}^{tB(\widetilde{v}_0)}\,\widetilde{v}_0$ to the initial value problems

$$\begin{aligned} v'(t) &= B(v_0)\,v(t)\,, \quad t \ge 0\,, \qquad v(0) = v_0\,,\\ \widetilde{v}'(t) &= B(\widetilde{v}_0)\,\widetilde{v}(t)\,, \quad t \ge 0\,, \qquad \widetilde{v}(0) = \widetilde{v}_0\,. \end{aligned}$$

Consequently, taking the difference and rewriting the right-hand side of the differential equation, we obtain

$$\big(v(t) - \widetilde{v}(t)\big)' = B(v_0)\,\big(v(t) - \widetilde{v}(t)\big) + \big(B(v_0) - B(\widetilde{v}_0)\big)\,\mathrm{e}^{tB(\widetilde{v}_0)}\,\widetilde{v}_0\,;$$

representing the solution by the variation-of-constants formula further yields

$$v(t) - \widetilde{v}(t) = \mathrm{e}^{tB(v_0)}\,\big(v_0 - \widetilde{v}_0\big) + \int_0^t \mathrm{e}^{(t-\tau)B(v_0)}\,\big(B(v_0) - B(\widetilde{v}_0)\big)\,\mathrm{e}^{\tau B(\widetilde{v}_0)}\,\widetilde{v}_0\,\mathrm{d}\tau\,.$$

It remains to estimate

$$\begin{aligned}\big\|v(t) - \widetilde{v}(t)\big\|_{H^m} &\leq \big\|\mathrm{e}^{tB(v_0)}\big\|_{H^m \leftarrow H^m} \, \|v_0 - \widetilde{v}_0\|_{H^m} \\ &\quad + \int_0^t \big\|\mathrm{e}^{(t-\tau)B(v_0)}\big\|_{H^m \leftarrow H^m} \big\|\big(B(v_0) - B(\widetilde{v}_0)\big)\, \mathrm{e}^{\tau B(\widetilde{v}_0)}\, \widetilde{v}_0\big\|_{H^m} \, \mathrm{d}\tau\,;\end{aligned}$$

by means of Lemma 2 and (B.4); finally, by applying the bound $1+x \leq \mathrm{e}^x$, the stated result follows. □

B.4. Derivatives. In the following, we are concerned with computing certain derivatives of the functions

$$\begin{aligned}\widehat{g}_1(\tau) &= \mathrm{e}^{(h-\,\tau)A}\, B\big(u(t_{n-1}+\tau)\big)\, \mathrm{e}^{\tau A}\, \widehat{u}_{n-1}\,, \\ \widehat{g}_2(\tau_1,\tau_2) &= \mathrm{e}^{(h-\,\tau_1)A}\, B\big(u(t_{n-1}+\tau_1)\big)\, \mathrm{e}^{(\tau_1-\,\tau_2)A}\, B\big(u(t_{n-1}+\tau_2)\big)\, \mathrm{e}^{\tau_2 A}\, \widehat{u}_{n-1}\,, \\ G_j(\tau) &= B\big(u(t_{n-1}+c_j\,\tau)\big) - B\big(\widehat{U}_{nj}(\tau)\big)\,, \qquad j=1,2\,,\end{aligned}$$

that are needed in Section 6 in order to derive the estimate (6.8) for the local error of the Strang type splitting method (3.2), see (6.2b), and (6.7e); for the convenience of the reader, we further recall the definitions

$$\begin{gathered}A = -\,\tfrac{1}{2}\,\mathrm{i}\,\big(-\Delta_\gamma + V_\gamma\big) = \tfrac{1}{2}\,\mathrm{i}\sum_{j=1}^{d}\gamma_j\,\big(\partial_{\xi_j}^2 - x_j^2\big)\,, \qquad B(v) = -\,\mathrm{i}\,\big(W + \vartheta\,|v|^2\big)\,, \\ \widehat{U}_{n1}(\tau) = \mathrm{e}^{a_1\tau A}\,\widehat{u}_{n-1}\,, \qquad \widehat{U}_{n2}(\tau) = \mathrm{e}^{a_2\tau A}\;\mathrm{e}^{\,b_1\tau B(\widehat{U}_{n1}(\tau))}\,\widehat{U}_{n1}(\tau)\,,\end{gathered}$$

see also (2.2) and (6.4). Henceforth, for linear operators K and L, we employ the commutator notation $[L,K] = LK - KL$.

Derivatives of B. In order to determine the Fréchet derivative of $B(v)$, we consider $B(v+w) - B(v) = -\,\mathrm{i}\,\vartheta\,\big(\overline{v}\,w + v\,\overline{w} + \overline{w}\,w\big)$ and thus obtain

$$\big(B'(v)\big)(w) = -\,\mathrm{i}\,\vartheta\,\big(\overline{v}\,w + v\,\overline{w}\big) = -\,2\,\mathrm{i}\,\vartheta\,\Re\big(\overline{v}\,w\big)\,. \tag{B.5a}$$

Consequently, it follows $\big(B'(v)\big)\big(w\,v\big) = 0$ for any function w with purely imaginary values. We next determine $\big(B'(v+w)\big)(\widetilde{w}) - \big(B'(v)\big)(\widetilde{w}) = -\,2\,\mathrm{i}\,\vartheta\,\Re\big(\overline{w}\,\widetilde{w}\big)$; this yields

$$\big(B''(v)\big)(w,\widetilde{w}) = -\,2\,\mathrm{i}\,\vartheta\,\Re\big(\overline{w}\,\widetilde{w}\big)\,.$$

As a consequence, for a function $v = v(\tau)$, it holds

$$\begin{aligned}\partial_\tau B(v) &= B'(v)(\partial_\tau v) = -\,2\,\mathrm{i}\,\vartheta\,\Re\big(\overline{v}\,\partial_\tau v\big)\,, \\ \partial_\tau^2\, B(v) &= B''(v)(\partial_\tau v, \partial_\tau v) + B'(v)(\partial_\tau^2\, v) = -\,2\,\mathrm{i}\,\vartheta\,\Big(|\partial_\tau v|^2 + \Re\big(\overline{v}\,\partial_\tau^2\, v\big)\Big)\,.\end{aligned} \tag{B.5b}$$

In particular, for $u = u(\tau)$ being the solution of (2.2), we employ the identities

$$\begin{aligned}\partial_\tau u &= \big(A + B(u)\big)\,u\,, \\ \partial_\tau^2 u &= \Big(B'(u)\big(A\,u + B(u)\,u\big)\Big)\,u + \big(A + B(u)\big)^2\,u\,,\end{aligned} \tag{B.5c}$$

in order to determine (B.5b).

Derivatives of $\widehat{g}_j$. On the one hand, differentiating $\widehat{g}_1$ twice, it follows

$$\begin{aligned}\partial_\tau^2\,\widehat{g}_1(\tau) &= \partial_\tau\Big(\mathrm{e}^{(h-\tau)A}\Big(-\big[A,B\big(u(t_{n-1}+\tau)\big)\big]+\partial_\tau B\big(u(t_{n-1}+\tau)\big)\Big)\,\mathrm{e}^{\tau A}\,\widehat{u}_{n-1}\Big)\\ &= \mathrm{e}^{(h-\tau)A}\Big(\Big[A,\big[A,B\big(u(t_{n-1}+\tau)\big)\big]\Big]-\,2\,\big[A,\partial_\tau B\big(u(t_{n-1}+\tau)\big)\big]\\ &\qquad+\partial_\tau^2 B\big(u(t_{n-1}+\tau)\big)\Big)\,\mathrm{e}^{\tau A}\,\widehat{u}_{n-1}\,.\end{aligned}$$

In a similar manner, we obtain

$$\begin{aligned}\partial_{\tau_1}\widehat{g}_2(\tau_1,\tau_2) &= \mathrm{e}^{(h-\tau_1)A}\Big(-\big[A,B\big(u(t_{n-1}+\tau_1)\big)\big]+\partial_{\tau_1}B\big(u(t_{n-1}+\tau_1)\big)\Big)\\ &\qquad\times\,\mathrm{e}^{(\tau_1-\tau_2)A}\,B\big(u(t_{n-1}+\tau_2)\big)\,\mathrm{e}^{\tau_2 A}\,\widehat{u}_{n-1}\,,\\ \partial_{\tau_2}\widehat{g}_2(\tau_1,\tau_2) &= \mathrm{e}^{(h-\tau_1)A}\,B\big(u(t_{n-1}+\tau_1)\big)\,\mathrm{e}^{(\tau_1-\tau_2)A}\Big(-\big[A,B\big(u(t_{n-1}+\tau_2)\big)\big]\\ &\qquad+\partial_{\tau_2}B\big(u(t_{n-1}+\tau_2)\big)\Big)\,\mathrm{e}^{\tau_2 A}\,\widehat{u}_{n-1}\,.\end{aligned}$$

Derivatives of G_j. Meanwhile we write $u=u(t_{n-1}+c_j\,\tau)$ for short; further, we let $\big(\mathrm{e}^{a_2(\cdot)A}\big)(\tau)=\mathrm{e}^{a_2\tau A}$. In order to determine the first and second derivatives of G_j for $j=1,2$, due to $\partial_\tau G_j=B'(u)\,\big(\partial_\tau u\big)-B'\big(\widehat{U}_{nj}\big)\,\big(\partial_\tau\widehat{U}_{nj}\big)$ and

$$\begin{aligned}\partial_\tau^2\,G_j &= B''(u)\,\big(\partial_\tau u,\partial_\tau u\big)-B''\big(\widehat{U}_{nj}\big)\,\big(\partial_\tau\widehat{U}_{nj},\partial_\tau\widehat{U}_{nj}\big)\\ &\qquad+B'(u)\,\big(\partial_\tau^2\,u\big)-B'\big(\widehat{U}_{nj}\big)\,\big(\partial_\tau^2\,\widehat{U}_{nj}\big)\,,\end{aligned}\tag{B.6a}$$

it remains to determine the derivatives of u and $\widehat{U}_{nj}$. Similarly to (B.5c), we obtain

$$\begin{aligned}\partial_\tau u &= c_j\big(A+B(u)\big)\,u\,,\\ \partial_\tau^2 u &= c_j^2\Big(B'(u)\big(A\,u+B(u)\,u\big)\Big)\,u+c_j^2\big(A+B\big(u\big)\big)^2\,u\,;\end{aligned}$$

furthermore, we have $\partial_\tau\widehat{U}_{n1}=a_1A\,\widehat{U}_{n1}$, $\partial_\tau^2\widehat{U}_{n1}=a_1^2A^2\,\widehat{U}_{n1}$, and

$$\begin{aligned}\partial_\tau\widehat{U}_{n2} &= a_2A\,\widehat{U}_{n2}+\mathrm{e}^{a_2(\cdot)A}\,\mathrm{e}^{b_1(\cdot)B(\widehat{U}_{n1})}\Big(b_1B'\big(\widehat{U}_{n1}\big)\big(\partial_\tau\widehat{U}_{n1}\big)\,\widehat{U}_{n1}+\partial_\tau\widehat{U}_{n1}\Big)\,,\\ \partial_\tau^2\,\widehat{U}_{n2} &= a_2A\,\partial_\tau\widehat{U}_{n2}+\mathrm{e}^{a_2(\cdot)A}\,\Big(a_2A\,+b_1B'\big(\widehat{U}_{n1}\big)\big(\partial_\tau\widehat{U}_{n1}\big)\Big)\,\mathrm{e}^{b_1(\cdot)B(\widehat{U}_{n1})}\\ &\qquad\times\Big(b_1B'\big(\widehat{U}_{n1}\big)\big(\partial_\tau\widehat{U}_{n1}\big)\,\widehat{U}_{n1}+\partial_\tau\widehat{U}_{n1}\Big)+\mathrm{e}^{a_2(\cdot)A}\,\mathrm{e}^{b_1(\cdot)B(\widehat{U}_{n1})}\\ &\qquad\quad\times\Big(b_1\Big(B''\big(\widehat{U}_{n1}\big)\big(\partial_\tau\widehat{U}_{n1},\partial_\tau\widehat{U}_{n1}\big)+B'\big(\widehat{U}_{n1}\big)\big(\partial_\tau^2\,\widehat{U}_{n1}\big)\Big)\,\widehat{U}_{n1}\\ &\qquad\qquad+b_1B'\big(\widehat{U}_{n1}\big)\,\big(\partial_\tau\widehat{U}_{n1}\big)\,\partial_\tau\widehat{U}_{n1}+\partial_\tau^2\,\widehat{U}_{n1}\Big)\,.\end{aligned}$$

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