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ON SPLITTING METHODS FOR SCHRÖDINGER-POISSON AND CUBIC NONLINEAR SCHRÖDINGER EQUATIONS

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Abstract. We give an error analysis of Strang-type splitting integrators for nonlinear Schrödinger equations. For Schrödinger-Poisson equations with an H^4-regular solution, a first-order error bound in the H^1 norm is shown and used to derive a second-order error bound in the L_2 norm. For the cubic Schrödinger equation with an H^4-regular solution, first-order convergence in the H^2 norm is used to obtain second-order convergence in the L_2 norm. Basic tools in the error analysis are Lie-commutator bounds for estimating the local error and H^m-conditional stability for error propagation, where $m = 1$ for the Schrödinger-Poisson system and $m = 2$ for the cubic Schrödinger equation.

1. Introduction

In this paper we give an error analysis of the Strang splitting time integration method applied to nonlinear Schrödinger equations

$$i\frac{\partial\psi}{\partial t} = -\Delta\psi + V\psi\,, \qquad x \in \mathbf{R}^3,\ t > 0, \tag{1.1}$$

where

$$V = V[\psi] = \pm|\psi|^2 \tag{1.2}$$

in the case of the cubic nonlinear Schrödinger equation, and

$$-\Delta V = \pm|\psi|^2 \tag{1.3}$$

in the case of the Schrödinger-Poisson equations. The equations are considered with asymptotic boundary conditions $\lim_{|x|\to\infty}\psi(x,t) = 0$ and $\lim_{|x|\to\infty}V(x) = 0$. The Poisson equation in (1.3) is thus to be interpreted as giving V by the convolution with the fundamental solution of the negative Laplacian,

$$V = V[\psi] = \mp\Delta^{-1}|\psi|^2 := \pm\frac{1}{4\pi|x|} * |\psi|^2\,.$$

In both cases, the initial data is given as $\psi(x,0) = \psi_0(x)$ for $x \in \mathbf{R}^3$.

The cubic nonlinear Schrödinger equation arises as a model equation from several areas of physics; see, e.g., Sulem and Sulem [20]. The one-dimensional problem ($x \in \mathbf{R}$) is important in fiber optics; see Agrawal [1]. Schrödinger-Poisson equations (1.1), (1.3) (also known as the Hartree equation), and generalizations are basic

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equations in quantum transport; see, e.g., Brezzi, and Markowich [6] and Illner, Zweifel, and Lange [13]. The more elaborate Schrödinger-Poisson system considered there has the same mathematical difficulties as (1.1) with (1.3), so we restrict our attention to this simpler set of equations.

In this paper we study the approximation properties of a semi-discretization in time. The numerical integrator we consider is a Strang-type splitting method, yielding approximations ψ_n to $\psi(t_n)$ with $t_n = n\tau$ for a step size $\tau > 0$ via

$$\begin{aligned} \psi^-_{n+1/2} &= e^{\frac{i}{2}\tau\Delta}\psi_n, \\ \psi^+_{n+1/2} &= e^{-i\tau V[\psi^-_{n+1/2}]}\,\psi^-_{n+1/2}, \\ \psi_{n+1} &= e^{\frac{i}{2}\tau\Delta}\psi^+_{n+1/2}\,. \end{aligned} \tag{1.4}$$

Here, $e^{it\Delta}$ is the solution operator of the free Schrödinger equation, expressed in terms of Fourier transforms as $\mathcal{F}^{-1}e^{-it|\xi|^2}\mathcal{F}$ and approximately computed by FFT in a Fourier spectral method, whereas the exponential of V acts as a pointwise multiplication operator. Note that $|\psi^+_{n+1/2}| = |\psi^-_{n+1/2}|$ and hence $V[\psi^+_{n+1/2}] = V[\psi^-_{n+1/2}]$. Method (1.4) is therefore explicit and time-reversible. The method is the composition of the exact flows of the differential equations

$$i\frac{\partial\psi}{\partial t} = -\Delta\psi \qquad \text{and} \qquad i\frac{\partial\psi}{\partial t} = V[\psi]\psi\,.$$

Such splitting methods are widely used; see, e.g., the early references Strang [19] and Hardin and Tappert [11], the study of the split-step Fourier method for the cubic nonlinear Schrödinger equation by Weideman and Herbst [21] and its use in fiber optics as in Agrawal [1, Section 2.4], the use of splitting methods for the time-dependent Kohn-Sham equations (closely related to the above Schrödinger-Poisson equations) in time-dependent density functional theory by Appel and Gross [2], and the papers by Bao, Mauser, and Stimming [4] on the use in the Schrödinger-Poisson-$X\alpha$ model and by Bao, Jaksch, and Markowich [3] on the numerical solution of the Gross-Pitaevskii equation for Bose-Einstein condensation, which is closely related to the cubic nonlinear Schrödinger equation. We further refer to the review of splitting methods by McLachlan and Quispel [18].

To our knowledge, there is as yet no rigorous convergence result in the literature for the splitting method for the cubic nonlinear Schrödinger equation. We mention, however, the work by Besse, Bidégaray, and Descombes [5], where an error analysis is given for globally Lipschitz-continuous nonlinearities, which is not the case with the cubic nonlinearity considered here. For the Schrödinger-Poisson equation, a first-order L_2 error bound over a time interval $[0, T]$ with suitably small T for initial data in the Sobolev space H^2 has been shown by Fröhlich [8].

Here, we derive error bounds for the Strang splitting over any given finite time interval that are second-order accurate in the L_2 norm under the condition of H^4 spatial regularity. This is more stringent than the H^2 regularity needed for linear Schrödinger equations with a smooth bounded potential [14]. The higher regularity requirement for the nonlinear equations considered here is caused by a term $\Delta^2\psi$ in the double Lie commutator of $i\Delta$ with the nonlinearity, whereas in the linear case there is a cancellation of higher derivatives that leaves only second-order derivatives. It is also interesting to compare with finite-difference time-stepping methods such as the Crank-Nicholson method or the implicit midpoint rule, for which second-order error bounds involve bounds on the third time derivative of the solution, which would require H^6-spatial regularity.

We remark that Weideman and Herbst [21] report an instability phenomenon in the Strang splitting for the cubic Schrödinger equation for certain step sizes, caused by resonances between the linear part, which has its spectrum on the imaginary axis, and the nonlinearity. This instability can lead to an exponential error growth that is stronger than in the error propagation by the equation itself, and can thus impair the long-time behaviour of the method. It should be noted, however, that this potential long-time instability is not at odds with the finite-time stability and convergence results given here.

We restrict our attention in this paper to nonlinear Schrödinger equations (1.1) on the whole space $\mathbf{R}^3$. Our arguments would apply similarly to problems with periodic boundary conditions and in lower space dimension, and could be extended to nonlinear Schrödinger equations with other power nonlinearities.

We only study semi-discretization in time but we expect that the results extend to various types of full discretization, uniformly in the spatial discretization parameter. What needs to be checked is the discrete version of the Lie commutator bounds established in this paper for the spatially continuous case. Once such bounds are available, the theory extends to the fully discrete case without further ado. The same remark apparently applies to splitting methods for other nonlinear evolution equations such as the KdV equation, where similarly the scheme of proof given here becomes applicable once the necessary Lie bracket bounds are established.

Throughout the paper, $L_2 = L_2(\mathbf{R}^3)$ denotes the Hilbert space of Lebesgue square integrable functions, and $H^k = H^k(\mathbf{R}^3)$ is the Sobolev space of L_2-functions having all generalized derivatives up to order k in L_2. We denote the solution of (1.1) at time t by $\psi(t) = \psi(\cdot, t)$. The L_2 norm is preserved along the solution, and we assume it to be of unit norm: $\|\psi(t)\|_{L_2} = \|\psi_0\|_{L_2} = 1$.

The paper is organized as follows. In the first part (Sections 2 to 6) we consider the Schrödinger-Poisson equation (1.1), (1.3) and then, in Sections 7 and 8, we extend the results and techniques to the cubic Schrödinger equation. Sections 2 and 7 state the results of this paper. In Section 3 we give some inequalities related to the nonlinearity in the Schrödinger-Poisson equation. In Section 4 we prove the first-order error bound in the H^1 Sobolev norm for solutions in H^3, and in Section 5 this is used to show the second-order error bound in L_2 for H^4-regular solutions. Section 6 proves an H^2-regularity result of the numerical solution. Finally, Section 8 outlines the modifications in the proofs needed for the cubic Schrödinger equation.

PART A. SCHRÖDINGER-POISSON EQUATIONS

2. Error bounds for solutions in H^4: Statement of results

In this section we formulate error bounds in the H^1 and L_2 norm and state some related results. According to a result by Illner, Zweifel, and Lange [13], the Schrödinger-Poisson equation (1.1), (1.3) has a global strong solution: $\psi_0 \in H^2$ implies $\psi(t) \in H^2$ for all $t \geq 0$. The result can be extended to yield H^k regularity of solutions to H^k initial data for any $k \geq 2$ globally in time. We suppose that the solution $\psi(t)$ to the Schrödinger-Poisson equation (1.1), (1.3) is in H^4 for $0 \leq t \leq T$, and set

$$m_k = \max_{0 \leq t \leq T} \|\psi(t)\|_{H^k} \qquad \text{for} \quad k \leq 4.$$

Our main result concerning the error of the Strang-type splitting scheme (1.4) reads as follows.

Theorem 2.1. *Suppose that the exact solution $\psi(t)$ to the Schrödinger-Poisson equation* (1.1), (1.3) *is in H^4 for $0 \le t \le T$. Then, the numerical solution ψ_n given by the splitting scheme* (1.4) *for the Schrödinger-Poisson equation* (1.1), (1.3) *with step size $\tau > 0$ has a first-order error bound in H^1 and a second-order error bound in L_2,*

$$\begin{aligned} \|\psi_n - \psi(t_n)\|_{H^1} &\le C(m_3, T)\,\tau \\ \|\psi_n - \psi(t_n)\|_{L_2} &\le C(m_4, T)\,\tau^2 \end{aligned} \qquad \text{for} \;\; t_n = n\tau \le T\,.$$

The following auxiliary results are of independent interest. We write the step of the splitting scheme (1.4) briefly as

$$\psi_{n+1} = \Phi_\tau(\psi_n)\,.$$

Proposition 2.2 (H^1-conditional L_2- and H^1-stability)**.** *If $\psi, \phi \in H^1$ with*

$$\|\psi\|_{H^1} \le M_1, \qquad \|\phi\|_{H^1} \le M_1,$$

then

$$\begin{aligned} \|\Phi_\tau(\psi) - \Phi_\tau(\phi)\|_{L_2} &\le e^{c_0\tau}\, \|\psi - \phi\|_{L_2}, \\ \|\Phi_\tau(\psi) - \Phi_\tau(\phi)\|_{H^1} &\le e^{c_1\tau}\, \|\psi - \phi\|_{H^1}, \end{aligned}$$

where c_0, c_1 only depend on M_1.

Note that also the L_2-stability estimate depends on bounds in H^1. The proof of Theorem 2.1 therefore proceeds by first showing the H^1 error bound, which, in particular, establishes the required bound of the H^1 norm of numerical solutions. We then are in the position to prove the L_2 error bound using the H^1-conditional L_2-stability.

Proposition 2.3 (Local error in H^1)**.** *If $\psi_0 \in H^3$ with $\|\psi_0\|_{H^3} \le M_3$, then the error after one step of the method* (1.4) *is bounded in the H^1 norm by*

$$\|\psi_1 - \psi(\tau)\|_{H^1} \le C_3\tau^2\,,$$

where C_3 only depends on M_3.

Proposition 2.4 (Local error in L_2)**.** *If $\psi_0 \in H^4$ with $\|\psi_0\|_{H^4} \le M_4$, then the error after one step of the method* (1.4) *is bounded in the L_2 norm by*

$$\|\psi_1 - \psi(\tau)\|_{L_2} \le C_4\tau^3\,,$$

where C_4 only depends on M_4.

Proposition 2.5 (H^2 regularity of the numerical solution)**.** *If $\psi_0 \in H^2$ and*

$$\|\psi_n\|_{H^1} \le M_1 \qquad \text{for all } n \text{ with } n\tau \le T,$$

then in fact

$$\|\psi_n\|_{H^2} \le e^{c_2 n\tau}\|\psi_0\|_{H^2} \qquad \text{for } n\tau \le T,$$

where c_2 only depends on M_1.

3. Some inequalities

Hardy's inequality (e.g., [15], p. 350)

$$\int_{\mathbf{R}^3} \frac{|u(y)|^2}{|y|^2}\, dy \le 4 \int_{\mathbf{R}^3} |\nabla u(y)|^2\, dy \qquad (u \in H^1)$$

implies some further inequalities that play an important role in the following.

Lemma 3.1. *For $u \in H^1$ and $v, w \in L_2$,*

$$\|\Delta^{-1}(uv)w\|_{L_2} \le K_0\, \|u\|_{H^1}\, \|v\|_{L_2}\, \|w\|_{L_2}\,, \tag{3.1}$$

and for $u, v \in L_2$ and $w \in H^1$,

$$\|\Delta^{-1}(uv)w\|_{L_2} \le K_0\, \|u\|_{L_2}\, \|v\|_{L_2}\, \|w\|_{H^1}\,. \tag{3.2}$$

Proof. (a) Inequality (3.1) is essentially Lemma 3.3 of [13]. We have

$$\|\Delta^{-1}(uv)w\|_{L_2} \le \|\Delta^{-1}(uv)\|_{L_\infty}\, \|w\|_{L_2}$$

and further, using the Cauchy-Schwarz inequality and Hardy's inequality,

$$\begin{aligned} \|\Delta^{-1}(uv)\|_{L_\infty} &= \sup_x \int_{\mathbf{R}^3} \frac{u(x-y)v(x-y)}{4\pi|y|}\, dy \\ &\le \frac{1}{4\pi} \sup_x \Big(\int_{\mathbf{R}^3} \frac{|u(x-y)|^2}{|y|^2}\, dy\Big)^{1/2} \Big(\int_{\mathbf{R}^3} |v(x-y)|^2\, dy\Big)^{1/2} \\ &\le \frac{1}{2\pi}\, \|u\|_{H^1}\, \|v\|_{L_2}\,. \end{aligned}$$

(b) For the proof of (3.2) we use a duality argument. Using partial integration and the L_∞ bound of part (a), we obtain

$$\begin{aligned} \|\Delta^{-1}(uv)w\|_{L_2} &= \sup_{\|\phi\|_{L_2}=1} \int_{\mathbf{R}^3} \Delta^{-1}(uv)w\phi\, dx = \sup_{\|\phi\|_{L_2}=1} \int_{\mathbf{R}^3} uv\, \Delta^{-1}(w\phi)\, dx \\ &\le \|uv\|_{L_1} \sup_{\|\phi\|_{L_2}=1} \|\Delta^{-1}(w\phi)\|_{L_\infty} \le \|u\|_{L_2}\, \|v\|_{L_2}\, \frac{1}{2\pi}\, \|w\|_{H^1}\,, \end{aligned}$$

which yields the result with $K_0 = \frac{1}{2\pi}$. □

With the product rule of derivatives, Lemma 3.1 immediately yields the following bounds.

Lemma 3.2. *We have*

$$\|\Delta^{-1}(uv)w\|_{H^1} \le K_1\, (\|u\|_{H^1}\, \|v\|_{H^1}\, \|w\|_{L_2} + \|u\|_{H^1}\, \|v\|_{L_2}\, \|w\|_{H^1}) \tag{3.3}$$

for $u, v, w \in H^1$, and

$$\|\Delta^{-1}(uv)w\|_{H^2} \le K_2 \sum_{(k,\ell,m)} \|u\|_{H^k}\, \|v\|_{H^\ell}\, \|w\|_{H^m} \tag{3.4}$$

for $u, v, w \in H^2$, where the sum is over all permutations (k, ℓ, m) of $(0, 1, 2)$. □

For further inequalities concerning $\Delta^{-1}(uv)w$ we refer to Castella [7] and Illner, Zweifel, and Lange [13].

4. Proof of the first-order error bound in H^1

4.1. H^1-conditional stability: Proof of Proposition 2.2. (a) Since $e^{i\tau\Delta}$ preserves both the L_2 and the H^1 norm, we only need to compare $e^{-i\tau V[\psi]}\psi$ and $e^{-i\tau V[\phi]}\phi$, which are the solutions at time τ of the linear initial value problems

$$\begin{aligned} i\dot\theta &= V[\psi]\theta, \qquad \theta(0)=\psi,\\ i\dot\eta &= V[\phi]\eta, \qquad \eta(0)=\phi, \end{aligned}$$

with H^1 norms of ψ and ϕ bounded by M_1. We rewrite the difference of the right-hand sides as

$$\begin{aligned} V[\psi]\theta - V[\phi]\eta &= \Delta^{-1}|\psi|^2\cdot\theta - \Delta^{-1}|\phi|^2\cdot\eta\\ &= \Delta^{-1}\big(|\psi|^2-|\phi|^2\big)\,\theta + \Delta^{-1}|\phi|^2\,(\theta-\eta)\\ &= \Delta^{-1}\big((\psi-\phi)\overline{\psi}\big)\,\theta + \Delta^{-1}\big(\phi(\overline{\psi}-\overline{\phi})\big)\,\theta + \Delta^{-1}(\phi\overline{\phi})\,(\theta-\eta). \end{aligned}$$

(b) By Lemma 3.1, we thus obtain

$$\begin{aligned} \|V[\psi]\theta - V[\phi]\eta\|_{L_2} \le\; & K_0\,\|\psi-\phi\|_{L_2}\,\|\psi\|_{H^1}\,\|\theta\|_{L_2} + K_0\,\|\psi-\phi\|_{L_2}\,\|\phi\|_{H^1}\,\|\theta\|_{L_2}\\ & + K_0\,\|\phi\|_{H^1}\,\|\phi\|_{L_2}\,\|\theta-\eta\|_{L_2} \end{aligned}$$

and hence, recalling unit L^2 norms of ϕ and θ,

$$\|\theta(t)-\eta(t)\|_{L_2} \le \|\psi-\phi\|_{L_2} + 2K_0M_1t\,\|\psi-\phi\|_{L_2} + \int_0^t K_0M_1\,\|\theta(s)-\eta(s)\|_{L_2}\,ds\,,$$

so that by the Gronwall inequality,

$$\|e^{-i\tau V[\psi]}\psi - e^{-i\tau V[\phi]}\phi\|_{L_2} = \|\theta(\tau)-\eta(\tau)\|_{L_2} \le e^{c_0\tau}\,\|\psi-\phi\|_{L_2}$$

where c_0 depends on M_1.

(c) We proceed in the same way for the H^1 estimate, using now Lemma 3.2 (and recalling unit L_2 norms) for the estimate

$$\|V[\psi]\theta - V[\phi]\eta\|_{H^1} \le 2K_1\big(\|\phi\|_{H^1}+\|\theta\|_{H^1}\big)\,\|\psi-\phi\|_{H^1} + 2K_1\|\phi\|_{H^1}\,\|\theta-\eta\|_{H^1}\,.$$

Next we estimate the H^1 norm of $\theta(t)$. By Lemma 3.2 and unit L_2 norms, we have

$$\|V[\psi]\theta\|_{H^1} \le K_1\left(\|\psi\|_{H^1}^2 + \|\psi\|_{H^1}\,\|\theta\|_{H^1}\right)\,,$$

which yields, using the bound $\|\psi\|_{H^1}\le M_1$,

$$\|\theta(t)\|_{H^1} \le (1+K_1M_1t)\,\|\psi\|_{H^1} + \int_0^t M_1\,\|\theta(s)\|_{H^1}\,ds\,.$$

With the Gronwall inequality we thus obtain

$$\|e^{-itV[\psi]}\psi\|_{H^1} = \|\theta(t)\|_{H^1} \le e^{a_1t}\,\|\psi\|_{H^1}\,, \tag{4.1}$$

where a_1 only depends on M_1. With the above estimate of $\|V[\psi]\theta - V[\phi]\eta\|_{H^1}$ this gives

$$\begin{aligned} \|\theta(t)-\eta(t)\|_{H^1} \le\; & \|\psi-\phi\|_{H^1} + \int_0^t 2K_1M_1(1+e^{a_1s})\,\|\psi-\phi\|_{H^1}\,ds\\ & + \int_0^t 2K_1M_1\,\|\theta(s)-\eta(s)\|_{H^1}\,ds\,. \end{aligned}$$

Once again by the Gronwall inequality, we finally obtain

$$\|e^{-i\tau V[\psi]}\psi - e^{-i\tau V[\phi]}\phi\|_{H^1} = \|\theta(\tau)-\eta(\tau)\|_{H^1} \le e^{c_1\tau}\,\|\psi-\phi\|_{H^1}\,,$$

where c_1 only depends on M_1. □

4.2. **Commutator bound.** We consider the vector fields on dense subsets of H^1,

$$\widehat{T}(\psi) = i\Delta\psi\,, \qquad \widehat{V}(\psi) = -iV[\psi]\psi\,,$$

that appear in (1.1). Their Lie commutator

$$\begin{aligned}
&[\widehat{T},\widehat{V}](\psi) = \widehat{T}'(\psi)\widehat{V}(\psi) - \widehat{V}'(\psi)\widehat{T}(\psi)\\
&= i\Delta\big(-i\Delta^{-1}(\psi\overline{\psi})\psi\big) + i\Delta^{-1}(i\Delta\psi\,\overline{\psi})\psi + i\Delta^{-1}(\psi\overline{i\Delta\psi})\psi + i\Delta^{-1}(\psi\overline{\psi})i\Delta\psi\\
&= 2\Delta^{-1}(\nabla\psi\cdot\nabla\overline{\psi})\,\psi + 2\Delta^{-1}(\nabla\psi\,\overline{\psi})\cdot\nabla\psi + 2\Delta^{-1}(\psi\,\nabla\overline{\psi})\cdot\nabla\psi + 2\Delta^{-1}(\psi\overline{\Delta\psi})\psi
\end{aligned}$$

plays an essential role in the error estimate.

Lemma 4.1. *The commutator is bounded in H^1 by*

$$\|[\widehat{T},\widehat{V}](\psi)\|_{H^1} \le C\,\|\psi\|_{H^2}^3 + C\,\|\psi\|_{H^1}^2\,\|\psi\|_{H^3} \qquad \textit{for all}\ \ \psi\in H^3\,.$$

Proof. The bound follows by applying Lemma 3.2 to the terms in $[\widehat{T},\widehat{V}](\psi)$. We note that the first three terms can be estimated using only the H^2 norm, but the last term requires a stronger norm. □

The estimate of the local error is now obtained with a nonlinear version of the analysis of splitting methods by Jahnke and Lubich [14], similar to Lubich [17]; cf. also Kozlov, Kværnø and Owren [16] for another related technique.

4.3. **Preparation: Lie derivatives.** We use the calculus of Lie derivatives (see, e.g., [9, Sect. III.5] or [12, Sect. IV.1.4]). Since this formalism only relies on the differentiability and the semi-group property of the flow, it is applicable in the present infinite-dimensional setting as well as in the finite-dimensional case. For a vector field F on H^1, such as $\widehat{T}$ or $\widehat{V}$ or $\widehat{H} = \widehat{T} + \widehat{V}$, we denote by φ_F^t the flow at time t of the differential equation $\dot{\psi} = F(\psi)$, that is, $\varphi_F^t(v)$ is the solution at time t of this differential equation with initial value $\psi(0) = v$. We consider the Lie derivative D_F defined by

$$\big(D_F G\big)(v) = \frac{d}{dt}\Big|_{t=0} G(\varphi_F^t(v)) = G'(v)F(v)$$

for another vector field G on H^1 and $v\in H^1$, and we set

$$\Big(\exp(tD_F)G\Big)(v) = G(\varphi_F^t(v)).$$

In particular, for the identity Id, the flow is reproduced as $\exp(tD_F)\mathrm{Id}(v) = \varphi_F^t(v)$. We then have the rule

$$\frac{d}{dt}\exp(tD_F)G(v) = \Big(D_F\exp(tD_F)G\Big)(v) = \Big(\exp(tD_F)D_F G\Big)(v).$$

The commutator $[D_F, D_G] = D_F D_G - D_G D_F$ of the Lie derivatives of two vector fields F and G is the Lie derivative of the commutator of the vector fields in reversed order:

$$[D_F, D_G] = D_{[G,F]}.$$

4.4. **Local error: Proof of Proposition 2.3.** (a) For notational simplicity we write D_H, D_T, D_V instead of $D_{\widehat{H}}$, $D_{\widehat{T}}$, $D_{\widehat{V}}$, respectively. We start from the nonlinear variation-of-constants formula

$$\psi(\tau) = \exp(\tau D_H)\mathrm{Id}\,(\psi_0) = \exp(\tau D_T)\mathrm{Id}\,(\psi_0) + \int_0^\tau \exp((\tau - s)D_H)\, D_V\, \exp(sD_T)\mathrm{Id}\,(\psi_0)\, ds.$$

Using this formula once more for the expression under the integral, we obtain

$$\psi(\tau) = \exp(\tau D_T)\mathrm{Id}\,(\psi_0) + \int_0^\tau \exp((\tau - s)D_T)\, D_V\, \exp(sD_T)\mathrm{Id}\,(\psi_0)\, ds + r_1$$

with the remainder

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

On the other hand, in this notation the numerical solution reads

$$\psi_1 = \exp(\tfrac{1}{2}\tau D_T) \exp(\tau D_V) \exp(\tfrac{1}{2}\tau D_T)\mathrm{Id}\,(\psi_0),$$

and Taylor expansion $\exp(\tau D_V) = I + \tau D_V + \tau^2 \int_0^1 (1 - \theta) \exp(\theta\tau D_V) D_V^2\, d\theta$ gives

$$\psi_1 = \exp(\tau D_T)\mathrm{Id}\,(\psi_0) + \tau \exp(\tfrac{1}{2}\tau D_T) D_V \exp(\tfrac{1}{2}\tau D_T)\mathrm{Id}\,(\psi_0) + r_2$$

with the remainder

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

(b) The error now becomes

$$\begin{aligned} \psi_1 - \psi(\tau) \quad &= \quad \tau\, \exp(\tfrac{1}{2}\tau D_T) D_V \exp(\tfrac{1}{2}\tau D_T)\mathrm{Id}\,(\psi_0) \\ &\quad - \int_0^\tau \exp((\tau - s)D_T)\, D_V\, \exp(sD_T)\mathrm{Id}\,(\psi_0)\, ds + (r_2 - r_1), \end{aligned} \tag{4.2}$$

and hence the principal error term is just the quadrature error of the midpoint rule applied to the integral over $[0, \tau]$ of the function

$$f(s) = \exp((\tau - s)D_T)\, D_V\, \exp(sD_T)\mathrm{Id}\,(\psi_0). \tag{4.3}$$

We express the quadrature error in first-order Peano form,

$$\tau\, f(\tfrac{1}{2}\tau) - \int_0^\tau f(s)\, ds = \tau^2 \int_0^1 \kappa_1(\theta)\, f'(\theta\tau)\, d\theta$$

with the (scalar, bounded) Peano kernel κ_1 of the midpoint rule. Since

$$\begin{aligned} f'(s) \quad &= \quad -\exp((\tau - s)D_T)\, [D_T, D_V]\, \exp(sD_T)\mathrm{Id}\,(\psi_0) \\ &= \quad \exp((\tau - s)D_T)\, D_{[\widehat{T},\widehat{V}]}\, \exp(sD_T)\mathrm{Id}\,(\psi_0) \\ &= \quad e^{is\Delta}\, [\widehat{T}, \widehat{V}](e^{i(\tau-s)\Delta}\psi_0)\ , \end{aligned}$$

the commutator bound of Lemma 4.1 shows that the quadrature error is bounded by

$$\Big\| \tau\, f(\tfrac{1}{2}\tau) - \int_0^\tau f(s)\, ds \Big\|_{H^1} \le C\tau^2 \|\psi_0\|_{H^2}^3\, . \tag{4.4}$$

(c) Finally, we estimate the remainder terms. For $\|\psi_0\|_{H^1} \le M_1$, we now show that they are bounded by

$$\|r_1\|_{H^1} + \|r_2\|_{H^1} \le C_1\tau^2\,, \tag{4.5}$$

where C_1 only depends on M_1. From the definitions we have

$$\begin{aligned}\exp(\rho D_H)D_V\exp(\sigma D_T)D_V\exp(sD_T)\mathrm{Id}\,(\psi_0) &= e^{is\Delta}\widehat{V}'(e^{i\sigma\Delta}\psi(\rho))e^{i\sigma\Delta}\widehat{V}(\psi(\rho)),\\ \exp(\tfrac{1}{2}\tau D_T)\exp(\theta\tau D_V)D_V^2\exp(\tfrac{1}{2}\tau D_T)\mathrm{Id}\,(\psi_0) &= e^{i\tau\Delta/2}\widehat{V}'(\eta)\widehat{V}(\eta),\end{aligned}$$

where $\eta = e^{-i\theta\tau V[\phi]}\,\phi$ with $\phi = e^{i\tau\Delta/2}\psi_0$, with $\|\eta\|_{H^1} \le e^{a_1\tau}\,\|\psi_0\|_{H^1}$ by (4.1). Since Lemma 3.2 yields the bounds (for ψ of unit L_2 norm)

$$\|\widehat{V}(\psi)\|_{H_1} \le C\,\|\psi\|_{H^1}^2 \quad \text{and} \quad \|\widehat{V}'(\psi)\phi\|_{H_1} \le C\,\|\psi\|_{H^1}^2\,\|\phi\|_{H^1}\,, \tag{4.6}$$

we obtain the bound (4.5). □

4.5. **Proof of the H^1 error bound of Theorem 2.1.** The stated error bound follows from Propositions 2.2 and 2.3 with the standard argument of Lady Windermere's fan [10, Sect. II.3]. Note that the boundedness in H^1 required by the stability lemma, is ensured by induction by the H^1 error bound. □

5. Proof of the second-order error bound in L_2

5.1. Double-commutator bound.

Lemma 5.1. *The double commutator of $\widehat{T}$ with $\widehat{V}$ is bounded in L_2 by*

$$\|[\widehat{T},[\widehat{T},\widehat{V}]](\psi)\|_{L_2} \le C\,\|\psi\|_{H^4}^3 \qquad \textit{for all}\ \ \psi \in H^4.$$

Proof. Direct calculation shows that among a plethora of more harmless terms that can be bounded, by Lemmas 3.1 and 3.2, in terms of the H^3 or even H^2 norms, the double commutator contains also the term $4i\Delta^{-1}(\psi\Delta^2\overline{\psi})\psi$, which can be bounded in terms of the H^4 norm. □

5.2. **Local error in L_2: Proof of Proposition 2.4.** (a) We return to the error formula (4.2) and write the principal error term in second-order Peano form

$$\tau\, f(\tfrac{1}{2}\tau) - \int_0^\tau f(s)\,ds = \tau^3\int_0^1 \kappa_2(\theta)\,f''(\theta\tau)\,d\theta$$

with the Peano kernel κ_2 of the midpoint rule and f of (4.3). We have

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

and hence Lemma 5.1 shows that the quadrature error is bounded in L_2 by $C\tau^3\|\psi_0\|_{H^4}^3$.

(b) With the function

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

the remainder term can be expressed as

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

where, in the same way as in part (c) of Section 4.4, the remainders can be bounded by

$$\|\widetilde{r}_1\|_{L_2} + \|\widetilde{r}_2\|_{L_2} \le \widetilde{C}_2 \tau^3$$

with $\widetilde{C}_2$ depending only on $\|\psi_0\|_{H^2}$. The other two terms in $r_2 - r_1$ form the quadrature error of a first-order two-dimensional quadrature formula, and are therefore bounded by

$$\Big\| \frac{\tau^2}{2}\, g\Big(\frac{\tau}{2}, 0\Big) - \int_0^\tau \int_0^{\tau - s} g(s,\sigma)\, d\sigma\, ds \Big\|_{L_2} \le C\tau^3 \Big(\max \Big\| \frac{\partial g}{\partial s} \Big\|_{L_2} + \max \Big\| \frac{\partial g}{\partial \sigma} \Big\|_{L_2} \Big),$$

where the maxima are taken over the triangle $0 \le s \le \tau$, $0 \le \sigma \le \tau - s$. The partial derivatives of g,

$$\begin{aligned} \frac{\partial g}{\partial s}(s,\sigma) &= \exp((\tau - s - \sigma) D_T) D_{[\widehat{T},\widehat{V}]} \exp(\sigma D_T) D_V \exp(s D_T) \mathrm{Id}\,(\psi_0) \\ &\quad + \exp((\tau - s - \sigma) D_T) D_V \exp(\sigma D_T) D_{[\widehat{T},\widehat{V}]} \exp(s D_T) \mathrm{Id}\,(\psi_0), \\ \frac{\partial g}{\partial \sigma}(s,\sigma) &= \exp((\tau - s - \sigma) D_T) D_{[\widehat{T},\widehat{V}]} \exp(\sigma D_T) D_V \exp(s D_T) \mathrm{Id}\,(\psi_0)\,, \end{aligned}$$

only contain $\widehat{V}$ and the simple commutator $[\widehat{T}, \widehat{V}]$ and their derivatives. The L_2 norms of $\partial g/\partial s$ and $\partial g/\partial \sigma$ can therefore be bounded in terms of the H^2 norm of ψ_0 using (4.6) and the argument of the proof of Lemma 4.1. Together, this shows

$$\|r_2 - r_1\|_{L_2} \le C_2 \tau^3\,,$$

where C_2 only depends on $\|\psi_0\|_{H^2}$. Recalling the error formula (4.2) and combining the above bound with that of part (a) yields the result of Proposition 2.4. □

5.3. **Proof of the L_2 error bound of Theorem 2.1.** With the H^2 regularity of the exact solution, with the L_2 bound of the local error of Proposition 2.4, and with the H^1-conditional L_2-stability of Proposition 2.2 together with the H^1 bound of the numerical solution established in Section 4, the result is obtained with the standard argument of Lady Windermere's fan [10, Sect. II.3]. □

6. H^2 regularity: Proof of Proposition 2.5

Since $e^{i\tau\Delta}$ preserves the H^2 norm, we only need to bound the H^2 norm of $e^{-i\tau V[\phi]}\phi$ for $\phi \in H^2$, which is the solution at time τ of

$$i\dot\eta = V[\phi]\eta, \qquad \eta(0) = \phi.$$

By Lemma 3.2 and $\|\eta\|_{L_2} = \|\phi\|_{L_2} = 1$,

$$\|V[\phi]\eta\|_{H^2} \le K_2 \left(\|\phi\|_{H^1} \|\eta\|_{H^2} + \|\phi\|_{H^2} \|\eta\|_{H^1} + \|\phi\|_{H^2} \|\phi\|_{H^1} \right).$$

By (4.1) we have

$$\|\eta(t)\|_{H^1} \le e^{a_1 t}\, \|\phi\|_{H^1}\,,$$

where a_1 depends only on M_1. For the H^2 norm we then obtain

$$\|\eta(t)\|_{H^2} \le \|\phi\|_{H^2} + \int_0^t C_1 \left(\|\phi\|_{H^2} + \|\eta(s)\|_{H^2} \right) ds$$

where C_1 only depends on M_1, and hence once again by the Gronwall inequality,

$$\|\eta(t)\|_{H^2} \le e^{a_2 t} \|\phi\|_{H^2}$$

where again a_2 only depends on M_1. Combining these estimates yields Proposition 2.5. □

PART B. THE CUBIC NONLINEAR SCHRÖDINGER EQUATION

7. Error bounds for solutions in H^4: Statement of results

For the cubic nonlinear Schrödinger equation (1.1), (1.2) with solutions in H^4 similar results are obtained. We suppose that the solution $\psi(t)$ to the cubic Schrödinger equation (1.1), (1.2) is in H^4 for $0 \le t \le T$, and set

$$m_4 = \max_{0\le t\le T} \|\psi(t)\|_{H^4}\,.$$

Theorem 7.1. *The numerical solution ψ_n given by the splitting scheme* (1.4) *for the cubic nonlinear Schrödinger equation with step size $\tau > 0$ has a first-order error bound in H^2 and a second-order error bound in L_2,*

$$\begin{aligned} \|\psi_n - \psi(t_n)\|_{H^2} &\le C(m_4, T)\,\tau \\ \|\psi_n - \psi(t_n)\|_{L_2} &\le C(m_4, T)\,\tau^2 \end{aligned} \qquad \text{for } t_n = n\tau \le T\,.$$

We again write the step of the splitting scheme (1.4) briefly as

$$\psi_{n+1} = \Phi_\tau(\psi_n)\,.$$

Proposition 7.2 (H^2-conditional L_2-, H^1- and H^2-stability)**.** *If $\psi, \phi \in H^2$ with*

$$\|\psi\|_{H^2} \le M_2, \qquad \|\phi\|_{H^2} \le M_2,$$

then

$$\begin{aligned} \|\Phi_\tau(\psi) - \Phi_\tau(\phi)\|_{L_2} &\le e^{c_0\tau}\,\|\psi-\phi\|_{L_2}, \\ \|\Phi_\tau(\psi) - \Phi_\tau(\phi)\|_{H^1} &\le e^{c_1\tau}\,\|\psi-\phi\|_{H^1}, \\ \|\Phi_\tau(\psi) - \Phi_\tau(\phi)\|_{H^2} &\le e^{c_2\tau}\,\|\psi-\phi\|_{H^2}, \end{aligned}$$

where c_0, c_1, c_2 only depend on M_2.

Note that the L_2- and H^1-stability estimates depend on bounds in H^2.

Proposition 7.3 (Local error in H^2)**.** *If $\psi_0 \in H^4$ with $\|\psi_0\|_{H^4} \le M_4$, then the error after one step of the method* (1.4) *is bounded in the H^2 norm by*

$$\|\psi_1 - \psi(\tau)\|_{H^2} \le C_4\tau^2\,,$$

where C_4 only depends on M_4.

Proposition 7.4 (Local error in L_2)**.** *If $\psi_0 \in H^4$ with $\|\psi_0\|_{H^4} \le M_4$, then the error after one step of the method* (1.4) *is bounded in the L_2 norm by*

$$\|\psi_1 - \psi(\tau)\|_{L_2} \le C_4\tau^3\,,$$

where C_4 only depends on M_4.

There is also an analogue of Proposition 2.5 for the cubic nonlinear Schrödinger equation, inferring H^3-regularity of the numerical solution from bounds in H^2.

For the *one-dimensional* cubic nonlinear Schrödinger equation we would obtain also H^1-conditional stability (essentially because $H^1(\mathbf{R}) \subset L_\infty(\mathbf{R})$).

8. Outline of the proofs

The proof of Theorem 7.1 and the above propositions is analogous to the corresponding results for the Schrödinger-Poisson equation. Essentially, the operator Δ^{-1} is to be replaced by the identity operator in all formulas. The estimates of Lemma 3.1 need to be replaced by

$$\begin{aligned} \|uvw\|_{L_2} &\leq K_0\, \|u\|_{H^1}\, \|v\|_{H^1}\, \|w\|_{H^1}, \\ \|uvw\|_{L_2} &\leq K_0\, \|u\|_{L_2}\, \|v\|_{H^2}\, \|w\|_{H^2}\,. \end{aligned}$$

The first bound follows from the Sobolev embedding $H^1 \subset L_6$, and the second bound from the Sobolev embedding $H^2 \subset L_\infty$. We then have the further bounds

$$\begin{aligned} \|uvw\|_{H^1} &\leq K_1\, \|u\|_{H^1}\, \|v\|_{H^2}\, \|w\|_{H^2}, \\ \|uvw\|_{H^2} &\leq K_2\, \|u\|_{H^2}\, \|v\|_{H^2}\, \|w\|_{H^2}\,. \end{aligned}$$

The commutator bounds now become

$$\begin{aligned} \|[\widehat{T},\widehat{V}](\psi)\|_{H^2} &\leq C\|\psi\|_{H^4}^3, \\ \|[\widehat{T},[\widehat{T},\widehat{V}]](\psi)\|_{L_2} &\leq C\|\psi\|_{H^4}^3\,. \end{aligned}$$

With these bounds the results follow in the same way as before.

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