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ORDER ESTIMATES IN TIME OF SPLITTING METHODS FOR THE NONLINEAR SCHRÖDINGER EQUATION*

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Abstract. In this paper, we consider the nonlinear Schrödinger equation $u_t + i\Delta u - F(u) = 0$ in two dimensions. We show, by an operator-theoretic proof, that the well-known Lie and Strang formulae (which are splitting methods) are approximations of the exact solution of order 1 and 2 in time.

Key words. nonlinear Schrödinger equation, splitting methods

AMS subject classifications. 65M12, 35Q

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1. Introduction.

Let us consider the cubic nonlinear Schrödinger equation

$$\begin{cases} \dfrac{\partial u}{\partial t} + i\Delta u + i\varepsilon|u|^2 u = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}^2, \end{cases} \tag{1.1}$$

with $\varepsilon = \pm 1$. A large number of articles are devoted to the numerical study of this equation using many different time discretizations, with or without splitting. The later case is represented by Crank–Nicolson type [4], Runge–Kutta type [1], [12], symplectic (see, for example, [14], [15]), and relaxation [2] methods. Splitting methods are based on a decomposition of the flow of (1.1). More precisely, let us define the flow X^t of the linear Schrödinger equation

$$\begin{cases} \dfrac{\partial v}{\partial t} + i\Delta v = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ v(x,0) = v_0(x), & x \in \mathbb{R}^2, \end{cases}$$

and the flow Y^t for the differential equation

$$\begin{cases} \dfrac{\partial w}{\partial t} + i\varepsilon|w|^2 w = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ w(x,0) = w_0(x), & x \in \mathbb{R}^2. \end{cases}$$

The idea of splitting methods is to approximate the flow of (1.1) by combining the two flows X^t and Y^t. Two classical methods are the following: the Lie formula given by $Z^t_{\mathrm{L}} = X^t Y^t$ (or $Y^t X^t$) and the Strang formula [18] $Z^t_{\mathrm{S}} = X^{t/2} Y^t X^{t/2}$ (or $Y^{t/2} X^t Y^{t/2}$); we introduce these four definitions since it is sometimes better to exchange the role of X^t and Y^t when one of the two equations is nonsmooth [17].

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This leads to good numerical methods for the periodic problem since the linear part may be computed efficiently by the use of fast Fourier transforms and the nonlinear part is solved exactly [19], [20]. We are interested in showing that the Lie formula is a first order approximation of the flow of (1.1) and the Strang formula is a second order approximation of the flow of (1.1). This result could be obtained formally with the formal Lie algebra theory (explained in the book [14] and in [13]), but here we give a simple proof allowing us to have an idea of the size of the constants.

The linear case has already been studied in [11] and [7] and we extend these results to the nonlinear case.

Following an idea of Donnat [8], we restrict ourselves to the case where the nonlinearity is a Lipschitz function; this may be done by a truncation method on a time interval before a possible blow-up. Thus we consider u the solution to the continuous problem

$$\begin{cases} \dfrac{\partial u}{\partial t} + i\Delta u - F(u) = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}^2, \end{cases} \tag{1.2}$$

where we assume that F is a Lipschitz function with constant K such that $F(0) = 0$ and the first four derivatives of F are bounded. We introduce the flow S^t, associated with (1.2) (that is, $u(t,\cdot) = S^t u_0$), and the two flows X^t and Y^t, solutions to

$$\begin{cases} \dfrac{\partial v}{\partial t} + i\Delta v = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ v(x,0) = v_0(x), & x \in \mathbb{R}^2, \end{cases} \tag{1.3}$$

and

$$\begin{cases} \dfrac{\partial w}{\partial t} - F(w) = 0, & x \in \mathbb{R}^2\,,\ t > 0, \\ w(x,0) = w_0(x), & x \in \mathbb{R}^2. \end{cases} \tag{1.4}$$

In what follows, we call Z^t any of the four splitting schemes when there is no ambiguity. Let us also recall that the semigroup X^t is a unitary operator on all classical Sobolev spaces $H^s = H^s(\mathbb{R}^2)$, $s \in \mathbb{R}$. Let us quote the main result of this article.

THEOREM 4.1. *For all u_0 in H^2 and for all $T > 0$, there exists C and h_0 such that for all $h \in (0, h_0]$, for all n such that $nh \le T$*

$$\left\| \left(Z_L^h\right)^n u_0 - S^{nh} u_0 \right\| \le C(\|u_0\|_{H^2}) h \|u_0\|_{H^2}.$$

Moreover, if u_0 belongs to H^4, then

$$\left\| \left(Z_S^h\right)^n u_0 - S^{nh} u_0 \right\| \le C(\|u_0\|_{H^4}) h^2 \|u_0\|_{H^4}.$$

To prove the convergence order for each splitting scheme, for a small $h > 0$ and all integer n such that $nh \le T$, we have to estimate the quantity $\|(Z^h)^n u_0 - S^{nh} u_0\|$, where $\|\cdot\|$ denotes the L^2 norm. As noticed in [5], the triangle inequality yields

$$\|(Z^h)^n u_0 - S^{nh} u_0\| \le \sum_{j=0}^{n-1} \|(Z^h)^{n-j-1} Z^h S^{jh} u_0 - (Z^h)^{n-j-1} S^{(j+1)h} u_0\|.$$

In section 3 we prove that for all the studied schemes there exists a constant C_0 such that for w_0 and $w_0' \in L^2$ and all $t \in [0,1]$

$$\|Z^t w_0 - Z^t w_0'\| \leq (1 + C_0 t)\|w_0 - w_0'\|. \tag{1.5}$$

Therefore

$$\|(Z^h)^n u_0 - S^{nh} u_0\| \leq \sum_{j=0}^{n-1} (1 + C_0 h)^{n-j-1} \left\|(Z^h - S^h) S^{jh} u_0\right\|. \tag{1.6}$$

Thus we may restrict our study to the case for which at each time step the initial data are the same for the continuous model and the splitting scheme and is equal to $v_0 = S^{jh} u_0$. Classical results on solutions to the nonlinear Schrödinger equation allow us to state that $S^{jh} u_0$ is uniformly bounded in H^4 for $jh \leq T$. Now we may write a Duhamel formula for the continuous problem (1.2) that reads as

$$u(t) = X^t v_0 + \int_0^t X^{t-s} F(u(s))\, ds$$

and express the difference of the exact solution and the splitting solution $v(t) = Z^t v_0$ as

$$u(t) - v(t) = \int_0^t X^{t-s} \left[F(u(s)) - F(v(s))\right] ds + R(t),$$

where the fact that F is Lipschitz and X^t is unitary in L^2 leads to

$$\|u(t) - v(t)\| \leq K \int_0^t \|u(s) - v(s)\|\, ds + \|R(t)\|.$$

There remains to show that the remainder $R(t)$ may be estimated as $\|R(t)\| = O(t^{p+1})$ for t small and to use a Gronwall lemma to conclude that the scheme is of order p.

This paper is organized as follows: In section 2, we prove a Gronwall lemma and some estimates on X^t and Y^t. In section 3, we show that each scheme is Lipschitz continuous and we study the local error between Z^t and S^t. Section 4 is devoted to the proof of Theorem 4.1.

2. Some useful estimates.

2.1. A Gronwall lemma.

LEMMA 2.1 (Gronwall). *Let P be a polynomial with positive coefficients and no constant term. We assume that the function ϕ is such that there exists a constant $C \geq 0$ such that for all $t \geq 0$*

$$0 \leq \phi(t) \leq \phi(0) + P(t) + C \int_0^t \phi(s) ds.$$

Then for all $\alpha > 1$ there exists $t_0 > 0$ such that for all $0 \leq t \leq t_0$

$$\phi(t) \leq \phi(0) e^{Ct} + \alpha P(t).$$

Proof. Let us set

$$\psi(t) = \left(\phi(0) + P(t) + C \int_0^t \phi(s) ds\right) e^{-Ct}.$$

Then

$$\psi'(t) = \left(P'(t) + C\phi(t) - C\left(\phi(0) + P(t) + C\int_0^t \phi(s)ds\right)\right)e^{-Ct} \leq P'(t)e^{-Ct};$$

therefore,

$$\psi(t) - \psi(0) \leq \int_0^t P'(s)e^{-Cs}ds,$$

and since $P(0) = 0$, $\psi(0) = \phi(0)$. Hence, because P' is positive,

$$\phi(t) \leq \psi(t)e^{Ct} \leq \phi(0)e^{Ct} + \int_0^t P'(s)e^{C(t-s)}\ ds \leq \phi(0)e^{Ct} + e^{Ct_0}\int_0^t P'(s)\ ds.$$

We choose t_0 such that $e^{Ct_0} \leq \alpha$ and, for all $0 \leq t \leq t_0$,

$$\phi(t) \leq \phi(0)e^{Ct} + \alpha P(t). \qquad \square$$

2.2. Estimates on the Schrödinger flow X^t. From the definition of the Schrödinger flow we first state that

$$\dot{X}^t = i\Delta X^t = iX^t\Delta. \tag{2.1}$$

This leads to the following estimates.

LEMMA 2.2. 1. *For all $w \in H^2$ and all $t \geq 0$,*

$$\|X^t w - w\| \leq t\|w\|_{H^2}. \tag{2.2a}$$

2. *For all $w \in H^4$ and all $t \geq 0$,*

$$\|X^t w - w\|_{H^2} \leq t\|w\|_{H^4}. \tag{2.2b}$$

3. *Let $T > 0$; there exists a constant C such that, for all $w \in \mathcal{C}^1([0,T]; H^2) \cap L^\infty([0,T], H^4)$ and $0 \leq t \leq T$,*

$$\left\|\int_0^t \left(X^{t-s}w(s) - X^{t/2}w(s)\right)ds\right\| \leq Ct^3(\|w\|_{\mathcal{C}^1([0,T];H^2)} + \|w\|_{L^\infty([0,T],H^4)}). \tag{2.2c}$$

4. *There exists a constant C such that for all $w \in H^4$,*

$$\left\|X^{t/2}w - \frac{1}{2}X^t w - \frac{1}{2}w\right\| \leq Ct^2\|w\|_{H^4}. \tag{2.2d}$$

Proof. 1. Let $w \in H^2$; we have

$$\|X^t w - w\| = \left\|\int_0^t \dot{X}^s w\ ds\right\| = \left\|\int_0^t X^s\Delta w\ ds\right\| \leq \int_0^t \|\Delta w\|ds \leq t\|w\|_{H^2}.$$

2. If we assume that $w \in H^4$, the estimate may be proved as the previous one replacing the L^2 norm by the H^2 norm.

3. A Taylor expansion gives

$$X^{t-s} - X^{t/2} = (t/2 - s)\dot{X}^{t/2} + \int_{t/2}^{t-s}(t - s - \sigma)\ddot{X}^\sigma\ d\sigma$$

and

$$(X^{t-s} - X^{t/2})w(s) = i(t/2 - s)X^{t/2}\Delta w(s) - \int_{t/2}^{t-s} (t - s - \sigma)X^{\sigma}\Delta^2 w(s)\ d\sigma.$$

A simple change of variables implies that

$$\int_0^t (t/2 - s)\Delta w(s)\ ds = \int_0^{t/2} (t/2 - s)[\Delta w(s) - \Delta w(t - s)]\ ds.$$

The Lipschitz constant of the map $s \mapsto \Delta w(s)$ is estimated using $\|w\|_{\mathcal{C}^1([0,T],H^2)}$ and, therefore,

$$\begin{aligned}
&\left\| \int_0^t \left(X^{t-s}w(s) - X^{t/2}w(s) \right) ds \right\| \\
&\quad \le \left\| \int_0^{t/2} (t/2 - s)[\Delta w(s) - \Delta w(t - s)]\ ds \right\| + \left\| \int_0^t \int_{t/2}^{t-s} (t - s - \sigma)X^{\sigma}\Delta^2 w(s) d\sigma ds \right\| \\
&\quad \le 2\|w\|_{\mathcal{C}^1([0,T],H^2)} \int_0^{t/2} (t/2 - s)^2 ds + \|w\|_{L^\infty([0,T],H^4)} \int_0^t \int_{t/2}^{t-s} (t - s - \sigma)\ d\sigma\ ds \\
&\quad \le Ct^3(\|w\|_{\mathcal{C}^1([0,T],H^2)} + \|w\|_{L^\infty([0,T],H^4)}).
\end{aligned}$$

4. Once more, Taylor expansions yield

$$X^{t/2} - \frac{1}{2}X^t - \frac{1}{2}X^0 = -\frac{1}{2}\int_0^{t/2} \sigma(\ddot{X}^{\sigma} + \ddot{X}^{t-\sigma})\ d\sigma,$$

and the same arguments as for the last estimates show the result. ∎

2.3. Estimates on the nonlinear flow Y^t. The definition of the nonlinear flow Y^t may also read as

$$Y^t w = w + \int_0^t F(Y^s w)\ ds. \tag{2.3}$$

LEMMA 2.3. *Let $w \in H^2$; then there exists a constant C that depends only on $M = \|w\|_\infty$ such that for all $0 \le t \le 1$*

$$\|Y^t w\| \le e^{Kt}\|w\| \text{ and } \|Y^t w\|_{H^2} \le C\|w\|_{H^2}. \tag{2.4a}$$

Moreover, if $w \in H^4$, then there exists a constant C that depends only on $M = \|w\|_\infty$ such that for all $0 \le t \le 1$

$$\|Y^t w\|_{H^4} \le C\|w\|_{H^4}. \tag{2.4b}$$

Finally, for w_1, $w_2 \in L^2$, there exists a constant C that depends only on F such that for all $0 \le t \le 1$

$$\|Y^t w_1 - Y^t w_2\| \le (1 + Ct)\|w_1 - w_2\|. \tag{2.4c}$$

Proof. Equation (2.3) first yields a L^∞ estimate, namely,

$$\|Y^t w\|_\infty \le \|w\|_\infty + K\int_0^t \|Y^s w\|_\infty\ ds.$$

Then the classical Gronwall lemma leads to

$$\|Y^t w\|_\infty \leq e^{Kt}\|w\|_\infty.$$

A L^2 estimate also follows from (2.3):

$$\|Y^t w\| \leq \|w\| + K\int_0^t \|Y^s w\|\ ds. \tag{2.5}$$

For all first order differential operators D

$$DY^t w = Dw + \int_0^t F'(Y^s w)D(Y^s w)\ ds,$$

and, denoting by M' the maximum for F', we obtain

$$\|DY^t w\| \leq \|Dw\| + M'\int_0^t \|DY^s w\|\ ds.$$

Differentiating once more,

$$\Delta Y^t w = \Delta w + \int_0^t \left(F''(Y^s w)D(Y^s w)^2 + F'(Y^s w)\Delta Y^s w\right) ds,$$

and, denoting by M'' the maximum for F'',

$$\|\Delta Y^t w\| \leq \|\Delta w\| + \int_0^t \left(M''\|DY^s w\|^2 + M'\|\Delta Y^s w\|\right) ds.$$

Using the Gagliardo–Nirenberg inequality,

$$\|DY^s w\|^2 \leq \|Y^s w\|_{H^2}\|Y^s w\|_\infty$$

and

$$\|\Delta Y^t w\| \leq \|\Delta w\| + \int_0^t \left(M''\|Y^s w\|_\infty + M'\right)\|Y^s w\|_{H^2}\ ds.$$

Therefore, using the L^∞ estimate, there exists a constant c such that

$$\|Y^t w\|_{H^2} \leq \|w\|_{H^2} + c\int_0^t \left(1 + e^{Ks}\right)\|Y^s w\|_{H^2}\ ds.$$

Last, using the Gronwall lemma,

$$\|Y^t w\|_{H^2} \leq \|w\|_{H^2}\exp\left(c\int_0^t \left(1 + e^{Ks}\right) ds\right).$$

Equation (2.5) also leads to

$$\|Y^t w\| \leq e^{Kt}\|w\|.$$

For $t \leq 1$, there exists a constant C such that

$$\exp\left(c\int_0^t \left(1 + e^{Ks}\right) ds\right) \leq C$$

and estimate (2.4a) follows. The proof for (2.4b) is similar and left to the reader. Finally, estimate (2.4c) is a simple consequence of the Gronwall lemma. ∎

3. Lipschitz properties of Z^t and local errors. In this section we more specifically give precise estimates for Lie and Strang formulae. We first show Lipschitz properties on Z^t, i.e., that estimate (1.5) is valid. Next we estimate the remainder $R(t)$ defined in the introduction.

3.1. Lipschitz properties.

- *Lie approximation—case $Z^t = X^t Y^t$.*
  The solution to the Lie approximation with initial data $v_0 \in L^2$ reads as

$$v(t) = Z^t v_0 = X^t v_0 + \int_0^t X^t F(Y^s v_0)\, ds.$$

  Therefore the difference between two solutions for initial data w_0 and w_0' in L^2 is

$$Z^t w_0 - Z^t w_0' = X^t(w_0 - w_0') + \int_0^t X^t(F(Y^s w_0) - F(Y^s w_0'))\, ds,$$

  and using the fact that X^t is unitary in L^2, that F is Lipschitz, and estimate (2.4c), we obtain that there exists a constant C depending only on F such that for $0 \le t \le 1$

$$\|Z^t w_0 - Z^t w_0'\| \le (1 + Ct)\|w_0 - w_0'\|.$$

- *Lie approximation—case $Z^t = Y^t X^t$.*
  Since

$$v(t) = Z^t v_0 = X^t v_0 + \int_0^t F(Y^s X^t v_0)\, ds,$$

  the difference is

$$Z^t w_0 - Z^t w_0' = X^t(w_0 - w_0') + \int_0^t (F(Y^s X^t w_0) - F(Y^s X^t w_0'))\, ds;$$

  thus, using the same tools as above, we obtain that there exists a constant C depending only on F such that for $0 \le t \le 1$

$$\|Z^t w_0 - Z^t w_0'\| \le (1 + Ct)\|w_0 - w_0'\|.$$

- *Strang approximation—case $Z^t = X^{t/2} Y^t X^{t/2}$.*
  Since

$$v(t) = Z^t v_0 = X^t v_0 + \int_0^t X^{t/2} F(Y^s X^{t/2} v_0)\, ds,$$

  we have

$$\begin{aligned} Z^t w_0 - Z^t w_0' &= X^t(w_0 - w_0') \\ &\quad + \int_0^t X^{t/2}(F(Y^s X^{t/2} w_0) - F(Y^s X^{t/2} w_0'))\, ds, \\ \|Z^t w_0 - Z^t w_0'\| &\le (1 + Ct)\|w_0 - w_0'\|. \end{aligned}$$

- *Strang approximation—case* $Z^t = Y^{t/2}X^tY^{t/2}$.
  Since

$$v(t) = Z^t v_0 = X^t Y^{t/2} v_0 + \int_0^{t/2} F(Y^s X^t Y^{t/2} v_0)\, ds,$$

  we have

$$\begin{aligned} Z^t w_0 - Z^t w_0' &= X^t Y^{t/2} w_0 - X^t Y^{t/2} w_0' \\ &\quad + \int_0^{t/2} (F(Y^s X^t X^{t/2} w_0) - F(Y^s X^t Y^{t/2} w_0'))\, ds, \\ \|Z^t w_0 - Z^t w_0'\| &\le (1 + Ct)\|w_0 - w_0'\|. \end{aligned}$$

3.2. Local errors.

- *Lie approximation—case* $Z^t = X^tY^t$.
  For $v_0 \in H^2$ and $0 \le t \le 1$, the remainder can be written as

$$R(t) = \int_0^t X^{t-s} F(X^s Y^s v_0)\, ds - \int_0^t X^t F(Y^s v_0)\, ds.$$

  Let us define $R_1(s) = F(X^sY^sv_0) - X^sF(Y^sv_0)$; then, using the fact that F is Lipschitz and estimates (2.2a) and (2.4a),

$$\begin{aligned} R_1(s) &= F(X^sY^sv_0) - F(Y^sv_0) + F(Y^sv_0) - X^sF(Y^sv_0), \\ \|R_1(s)\| &\le K\|X^sY^sv_0 - Y^sv_0\| + \|F(Y^sv_0) - X^sF(Y^sv_0)\| \\ &\le s\,(K\|Y^sv_0\|_{H^2} + \|F(Y^sv_0)\|_{H^2}) \\ &\le Cs\|v_0\|_{H^2}. \end{aligned}$$

  Therefore, since $R(t) = \int_0^t X^{t-s}R_1(s)ds$,

$$\|R(t)\| \le C\|v_0\|_{H^2} \int_0^t s\, ds = \frac{Ct^2}{2}\|v_0\|_{H^2}.$$

- *Lie approximation—case* $Z^t = Y^tX^t$.
  For $v_0 \in H^2$ and $0 \le t \le 1$, the remainder can be written as

$$R(t) = \int_0^t X^{t-s} F(Y^s X^s v_0)\, ds - \int_0^t F(Y^s X^t v_0)\, ds.$$

  In this case $R(t) = \int_0^t R_1(s)ds$, where $R_1 = X^{t-s}F(Y^sX^sv_0) - F(Y^sX^tv_0)$, and using the fact that F is Lipschitz and estimates (2.2a), (2.4a), (2.4c), we obtain

$$\begin{aligned} R_1(s) &= X^{t-s}F(Y^sX^sv_0) - F(Y^sX^sv_0) + F(Y^sX^sv_0) - F(Y^sX^tv_0), \\ \|R_1(s)\| &\le (t-s)\|F(Y^sX^sv_0)\|_{H^2} + K\|X^sv_0 - X^tv_0\| \\ &\le C(t-s)\|v_0\|_{H^2}; \end{aligned}$$

  hence

$$\|R(t)\| \le C\|v_0\|_{H^2} \int_0^t (t-s)\, ds = \frac{Ct^2}{2}\|v_0\|_{H^2}.$$

- *Strang approximation—case* $Z^t = X^{t/2}Y^tX^{t/2}$.
  For $v_0 \in H^4$ and $0 \le t \le 1$, the remainder can be written as

$$R(t) = \int_0^t X^{t-s}F(X^{s/2}Y^sX^{s/2}v_0)\ ds - \int_0^t X^{t/2}F(Y^sX^{t/2}v_0)\ ds.$$

We may write $R(t)$ as $R(t) = \int_0^t R_1(s)\ ds + X^{t/2}\int_0^t R_2(s)\ ds$, where

$$R_1(s) = X^{t-s}w(s) - X^{t/2}w(s), \qquad w(s) = F(Y^sX^{t/2}v_0),$$

and

$$R_2(s) = F(X^{s/2}Y^sX^{s/2}v_0) - F(Y^sX^{t/2}v_0).$$

Using estimate (2.2c), we obtain that

$$\left\| \int_0^t R_1(s)\ ds \right\| \le Ct^3\|v_0\|_{H^4}.$$

A Taylor expansion yields that

$$\begin{aligned} R_2(s) = {} & F'(v_0)\cdot(X^{s/2}Y^sX^{s/2}v_0 - Y^sX^{t/2}v_0) \\ & + \int_0^1 (1-\theta)\Big[F''(v_0 + \theta(X^{s/2}Y^sX^{s/2}v_0 - v_0)) \\ & \qquad\qquad \cdot (X^{s/2}Y^sX^{s/2}v_0 - v_0)^2 \\ & \quad - F''(v_0 + \theta(Y^sX^{t/2}v_0 - v_0))\cdot(Y^sX^{t/2}v_0 - v_0)^2\Big]d\theta. \end{aligned}$$

Using triangle inequalities, estimates (2.2a), (2.4a), formulation (2.3), and the fact that F is Lipschitz, we obtain that

$$\|X^{s/2}Y^sX^{s/2}v_0 - v_0\| \le Cs\|v_0\|_{H^2}$$

and

$$\|Y^sX^{t/2}v_0 - v_0\| \le Ct\|v_0\|_{H^2}.$$

Besides, we recall that F'' is uniformly bounded by M'', and therefore, using that H^2 is an algebra,

$$\begin{aligned} \Bigg\| \int_0^1 (1-\theta)\Big[& F''(v_0 + \theta(X^{s/2}Y^sX^{s/2}v_0 - v_0))\cdot(X^{s/2}Y^sX^{s/2}v_0 - v_0)^2 \\ & - F''(v_0 + \theta(Y^sX^{t/2}v_0 - v_0))\cdot(Y^sX^{t/2}v_0 - v_0)^2\Big]d\theta\Bigg\| \le Ct^2\|v_0\|_{H^4}^2. \end{aligned}$$

Moreover, let us define $R_3(s) = X^{s/2}Y^sX^{s/2}v_0 - Y^sX^{t/2}v_0$; formulation (2.3) yields that

$$\begin{aligned} R_3(s) = {} & X^sv_0 - X^{t/2}v_0 + \int_0^s (X^{s/2}F(Y^\sigma X^{s/2}v_0) - F(Y^\sigma X^{s/2}v_0))\ d\sigma \\ & + \int_0^s (F(Y^\sigma X^{s/2}v_0) - F(Y^\sigma X^{t/2}v_0))\ d\sigma. \end{aligned}$$

A simple change of variable in lemma (2.2c) proves that

$$\left\| \int_0^t (X^s v_0 - X^{t/2} v_0)\ ds \right\| \le C t^3 \|v_0\|_{H^4},$$

and using once more estimates (2.2a) and (2.4b) and the fact that F is Lipschitz, we have

$$\left\| \int_0^t \int_0^s (X^{s/2} F(Y^\sigma X^{s/2} v_0) - F(Y^\sigma X^{s/2} v_0))\ d\sigma ds \right\| \le C t^3 \|v_0\|_{H^2}$$

and, also using (2.2c),

$$\left\| \int_0^t \int_0^s (F(Y^\sigma X^{s/2} v_0) - F(Y^\sigma X^{t/2} v_0))\ d\sigma ds \right\| \le C t^3 \|v_0\|_{H^2}.$$

Finally, since $X^{t/2}$ is unitary,

$$\left\| X^{t/2} \int_0^t R_2(s)\ ds \right\| \le C t^3 \|v_0\|_{H^4},$$

and the conclusion is that

$$\|R(t)\| \le C(1 + \|v_0\|_{H^4}) t^3 \|v_0\|_{H^4}.$$

- *Strang approximation—case* $Z^t = Y^{t/2} X^t Y^{t/2}$.
  For $v_0 \in H^4$ and $0 \le t \le 1$, the remainder can be written as

$$\begin{aligned} R(t) = &\int_0^t X^{t-s} F(Y^{s/2} X^s Y^{s/2} v_0)\ ds \\ &-\frac{1}{2} \int_0^t X^t F(Y^{s/2} v_0)\ ds - \frac{1}{2} \int_0^t F(Y^{s/2} X^t Y^{t/2} v_0)\ ds. \end{aligned}$$

Taylor expansions yield

$$\begin{aligned} F(Y^{s/2} X^s Y^{s/2} v_0) &= F(v_0) + F'(v_0) \cdot (Y^{s/2} X^s Y^{s/2} v_0 - v_0) \\ &\quad + \int_0^1 (1-\theta) F''(v_0 + \theta(Y^{s/2} X^s Y^{s/2} v_0 - v_0)) \\ &\qquad \cdot (Y^{s/2} X^s Y^{s/2} v_0 - v_0)^2 d\theta, \\ F(Y^{s/2} v_0) &= F(v_0) + F'(v_0) \cdot (Y^{s/2} v_0 - v_0) \\ &\quad + \int_0^1 (1-\theta) F''(v_0 + \theta(Y^{s/2} v_0 - v_0)) \\ &\qquad \cdot (Y^{s/2} v_0 - v_0)^2 d\theta, \\ F(Y^{s/2} X^t Y^{t/2} v_0) &= F(v_0) + F'(v_0) \cdot (Y^{s/2} X^t Y^{t/2} v_0 - v_0) \\ &\quad + \int_0^1 (1-\theta) F''(v_0 + \theta(Y^{s/2} X^t Y^{t/2} v_0 - v_0)) \\ &\qquad \cdot (Y^{s/2} X^t Y^{t/2} v_0 - v_0)^2 d\theta, \end{aligned}$$

and the same sort of estimates as above give

$$\begin{aligned} \|Y^{s/2} X^s Y^{s/2} v_0 - v_0\| &\le C s \|v_0\|_{H^4}, \\ \|Y^{s/2} v_0 - v_0\| &\le C s \|v_0\|_{H^4}, \\ \|Y^{s/2} X^t Y^{t/2} v_0 - v_0\| &\le C t \|v_0\|_{H^4}. \end{aligned}$$

Therefore, the time integral over the interval $[0,t]$ of the integral remainders may be estimated by $Ct^3\|v_0\|_{H^2}^2$. Besides, there remains to estimate $\int_0^t R_1(s)\ ds$ with

$$\begin{aligned}R_1(s) = &\left(X^{t-s} - \frac{1}{2}X^t - \frac{1}{2}\mathrm{Id}\right)F(v_0)\\ &+ (X^{t-s} - \mathrm{Id})F'(v_0)\cdot(Y^{s/2}X^sY^{s/2}v_0 - v_0)\\ &- \frac{1}{2}(X^t - \mathrm{Id})F'(v_0)\cdot(Y^{s/2}v_0 - v_0)\\ &+ F'(v_0)\cdot(Y^{s/2}X^sY^{s/2}v_0 - v_0)\\ &- \frac{1}{2}F'(v_0)\cdot(Y^{s/2}v_0 - v_0) - \frac{1}{2}F'(v_0)\cdot(Y^{s/2}X^tY^{t/2}v_0 - v_0).\end{aligned}$$

The first term is estimated by $Ct^3\|v_0\|_{H^4}$, combining estimates (2.2c) and (2.2d). The two next terms are, respectively, estimated by $CM'(t-s)s\|v_0\|_{H^4}$ and $CM'ts\|v_0\|_{H^2}$.
Last, since $F'(v_0)$ is a linear operator, we have to study $\int_0^t F'(v_0)R_2(s)\ ds$ with

$$\begin{aligned}R_2(s) &= Y^{s/2}X^sY^{s/2}v_0 - \frac{1}{2}Y^{s/2}v_0 - \frac{1}{2}Y^{s/2}X^tY^{t/2}v_0\\ &= X^sv_0 + \frac{1}{2}\int_0^s X^sF(Y^{\sigma/2}v_0)\ d\sigma + \frac{1}{2}\int_0^s F(Y^{\sigma/2}X^sY^{s/2}v_0)\ d\sigma\\ &\quad - \frac{1}{2}v_0 - \frac{1}{4}\int_0^s F(Y^{\sigma/2}v_0)\ d\sigma\\ &\quad - \frac{1}{2}X^tv_0 - \frac{1}{4}\int_0^t X^tF(Y^{\sigma/2}v_0)\ d\sigma - \frac{1}{4}\int_0^t F(Y^{\sigma/2}X^tY^{t/2}v_0)\ d\sigma,\end{aligned}$$

where we have used intensively formulation (2.3). Everywhere where F occurs we subtract and add $F(v_0)$. This leads to terms involving differences which may be estimated by $Ct^2\|v_0\|_{H^2}$, and therefore their time integral is bounded by $Ct^3\|v_0\|_{H^2}$. The only terms that remain are $R_3(s) = X^sv_0 - \frac{1}{2}v_0 - \frac{1}{2}X^tv_0$ and $R_4(s) = \frac{1}{2}\int_0^s X^sF(v_0)d\sigma - \frac{1}{4}\int_0^t X^tF(v_0)d\sigma$. We have

$$R_3(s) = (X^sv_0 - X^{t/2}v_0) + \left(X^{t/2}v_0 - \frac{1}{2}v_0 - \frac{1}{2}X^tv_0\right),$$

$$\left\|\int_0^t R_3(s)\ ds\right\| \le Ct^3\|v_0\|_{H^4};$$

$$R_4(s) = \frac{1}{2}\left(s(X^s - X^t)F(v_0) + \left(s - \frac{t}{2}\right)X^tF(v_0)\right),$$

$$\left\|\int_0^t R_4(s)\ ds\right\| = \left\|\int_0^t s(X^s - X^t)F(v_0)\ ds\right\| \le Ct^3\|v_0\|_{H^2}.$$

Finally, we obtain that

$$\|R(t)\| \le C(1 + \|v_0\|_{H^4})t^3\|v_0\|_{H^4}.$$

This last estimate concludes the study of the remainders for the four schemes. Now a consequence of the Gronwall lemma 2.1 is the following lemma.

LEMMA 3.1. *Let $v_0 \in H^2$; there exists $t_0 > 0$ such that for all $0 \le t \le t_0$*

$$\|Z_{\mathrm{L}}^t v_0 - S^t v_0\| \le Ct^2,$$

where C depends on $\|v_0\|_{H^2}$. Moreover, if $v_0 \in H^4$, there exists $t_1 > 0$ such that for all $0 \le t \le t_1$

$$\|Z_{\mathrm{S}}^t v_0 - S^t v_0\| \le Ct^3,$$

where C depends on $\|v_0\|_{H^4}$.

Remark 3.2. In [11], Jahnke and Lubich have shown the first and second order approximation for a linear Schrödinger equation under the weaker regularity conditions $v_0 \in H^1$ and $v_0 \in H^2$. Unfortunately, it is not possible to keep exactly the same hypothesis for the nonlinear case for the following reason: Let us focus on the first order approximation; we can formally extend the results of Jahnke and Lubich in the nonlinear case using Lie commutators. However, the Lie commutator between the Laplace operator and the nonlinear term involves a term containing $(\partial v_0/\partial x)^2$ and $(\partial v_0/\partial y)^2$ (see [13] for more details). To control these two terms, we have two possibilities, either we assume that $v_0 \in H^2$ and we use a Gagliardo–Nirenberg inequality, or we assume that $v_0 \in H^1 \cap W^{1,+\infty}$. Thus, in our lemma, H^2 is not optimal if we also assume that $v_0 \in W^{1,+\infty}$.

4. Order estimate.

THEOREM 4.1. *For all u_0 in H^2 and for all $T > 0$, there exists C and h_0 such that for all $h \in (0, h_0]$, for all n such that $nh \le T$*

$$\left\| \left(Z_L^h\right)^n u_0 - S^{nh} u_0 \right\| \le C(\|u_0\|_{H^2}) h \|u_0\|_{H^2}.$$

Moreover, if u_0 belongs to H^4, then

$$\left\| \left(Z_S^h\right)^n u_0 - S^{nh} u_0 \right\| \le C(\|u_0\|_{H^4}) h^2 \|u_0\|_{H^4}.$$

Proof. As noticed in the introduction, the triangle inequality yields

$$\|(Z^h)^n u_0 - S^{nh} u_0\| \le \sum_{j=0}^{n-1} \|(Z^h)^{n-j-1} Z^h S^{jh} u_0 - (Z^h)^{n-j-1} S^{(j+1)h} u_0\|.$$

In section 3 we have proved that for all the studied schemes there exists a constant C_0 such that for w_0 and $w_0' \in L^2$ and all $t \in [0, 1]$

$$\|Z^t w_0 - Z^t w_0'\| \le (1 + C_0 t)\|w_0 - w_0'\|,$$

and therefore

$$\|(Z^h)^n u_0 - S^{nh} u_0\| \le \sum_{j=0}^{n-1} (1 + C_0 h)^{n-j-1} \|(Z^h - S^h) S^{jh} u_0\|.$$

For the Lie formula when u_0 belongs to H^2, for all j such that $jh \le T$, $S^{jh} u_0$ belongs to H^2 and is uniformly bounded in this space; thus we have

$$\|(Z_{\mathrm{L}}^h - S^h) S^{jh} u_0\| \le C(\|u_0\|_{H^2}) h^2 \|u_0\|_{H^2},$$

and we deduce that

$$\begin{aligned}\|(Z_{\mathrm{L}}^h)^n u_0 - S^{nh}u_0\| &\le C(\|u_0\|_{H^2})\|u_0\|_{H^2}\sum_{j=0}^{n-1}\exp(C_0h)^{n-j-1}h^2\\ &\le C(\|u_0\|_{H^2})\|u_0\|_{H^2}\exp(C_0T)nh^2\\ &\le C(\|u_0\|_{H^2})\|u_0\|_{H^2}h.\end{aligned}$$

For the scheme Z_{S}^h, when u_0 belongs to H^4, for all j such that $jh \le T$, $S^{jh}u_0$ belongs to H^4 and is uniformly bounded in this space, and we have

$$\begin{aligned}\|(Z_{\mathrm{S}}^h)^n u_0 - S^{nh}u_0\| &\le C(\|u_0\|_{H^4})\|u_0\|_{H^4}\sum_{j=0}^{n-1}\exp(C_0h)^{n-j-1}h^3\\ &\le C(\|u_0\|_{H^4})\|u_0\|_{H^4}\exp(C_0T)nh^3\\ &\le C(\|u_0\|_{H^4})\|u_0\|_{H^4}h^2.\end{aligned}$$

This concludes the proof of Theorem 4.1. □

Remark 4.2. Theorem 4.1 shows that the Lie and Strang formulae are approximations of order one and two of the exact solution. We can notice that the proof can be extended to high order splitting formulae. In [9], it is shown that we can construct Nth order approximation ($N \ge 3$) by considering splitting schemes of the form

$$Z_{\mathrm{HO}}^t = X^{c_0t}Y^{d_1t}X^{c_1t}Y^{d_2t}\cdots Y^{d_{m-1}t}X^{c_{m-1}t}Y^{d_mt}X^{c_mt}, \tag{4.1}$$

but we have to assume that at least one of the coefficient $c_0, \dots, c_m$ must be negative and at least one of the coefficient $d_1, \dots, d_m$ must be negative. (This result generalized the fundamental result of [16].) The same result holds if we consider convex combinations of (4.1). For these kinds of formulae, the Lipschitz property is an immediate consequence of their forms, and we notice that we can still use some Taylor formulae for X^t and Y^t to show that the remainder may be estimated as $\|R(t)\| = O(t^{N+1})$ for t small; however, as we have seen for the last scheme studied in the previous proof, it would be very technical.

5. Numerical experiments. We proved in the previous sections that the order p of Lie and Strang formulations are, respectively, 1 and 2 for initial data in H^2 and H^4.

If the numerical order p_{num} given in Table 5.1 does confirm the theoretical orders, it is nevertheless difficult to force the desired regularity for a discretized initial datum. Typically, the regularity of the L^2 initial datum in Figure 5.1 is certainly slightly better.

Let us define $t_n = nh$ and let $\Omega = [-10, 10] \times [-10, 10]$ be the computational domain. The numerical order p_{num} is computed by

$$p_{\mathrm{num}} = \max_{t_n\in[0,T]} \frac{1}{\ln 2}\ln\left(\frac{\|u_2 - u_1\|_{L^2(\Omega)}}{\|u_3 - u_2\|_{L^2(\Omega)}}\right),$$

where u_1 is computed for the time step h, and u_2 and u_3 are, respectively, computed for time steps $h/2$ and $h/4$.

We use initial data displayed in Figure 5.1, and in order to avoid numerical reflections due to boundaries we choose periodic boundary conditions and a FFT method to invert the Laplacian.

TABLE 5.1
Computation of p_{num} for different initial data.

	Lie	Strang
H^2	1.000685	2.000072
H^1	1.001721	2.006374
L^2	1.014480	2.010045

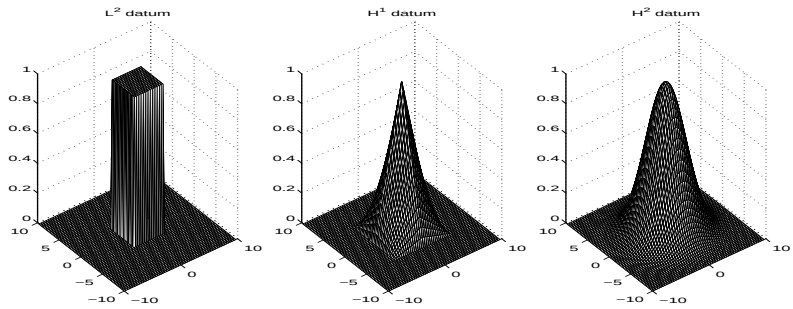

FIG. 5.1. *Initial data used for numerical experiments.*

TABLE 5.2
Computation of p_{num} for different time and space steps.

	$N = 64$	$N = 128$	$N = 256$
$h = 10^{-3}$	2.000016	2.000072	2.000289
$h = 10^{-2}$	2.001637	2.007160	2.030023

The results displayed in Table 5.1 are computed for $h = 10^{-3}$ and $N = 128$ points in both space dimensions.

This results are not much dependent on the choice for the time and space steps. Indeed, for the H^2 initial datum and the Strang formulation, we obtain the results of Table 5.2.

6. Conclusion. We have shown in this paper that, for the nonlinear Schrödinger equation, the Lie and Strang formulae are, respectively, approximations of order 1 and 2. This result could be extended to cover the case of the Schrödinger–Debye equations [3], where one can find a proof for the first order. The case of the nonlinear heat equation could also be treated with the same arguments because we have never used the group property but only the semigroup property of the flow of the linear Schrödinger equation; besides, we may write an equivalent of Lemma 2.2. In particular, this extends also the results of [6]. Our proof may also be extended to the Ginzburg–Landau equation, for which some splitting methods are also used (see, e.g., [10]) since it will use the fact that we are able to perform the proof for both the Schrödinger and the heat equation.

Our analysis does not give any hint on how to choose one splitting scheme among the others. The order of convergence is not the only criterion as stressed in the introduction: in case of stiff terms, the order of the different steps is of consequence. Namely, the last step should be the stiff one which is the nonlinear step Y^t in our context. This fact is hidden in our constants that depend on norms that grow with the size of the exact solution.

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