Avoiding order reduction when integrating nonlinear Schrödinger equation with Strang method

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Abstract

In this paper a technique is suggested to avoid order reduction when using Strang method to integrate nonlinear Schrödinger equation subject to time-dependent Dirichlet boundary conditions. The computational cost of this technique is negligible compared to that of the method itself, at least when the timestepsize is fixed. Moreover, a thorough error analysis is given as well as a modification of the technique which allows to conserve the symmetry of the method while retaining its second order.

Keywords: nonlinear Schrödinger equation, Strang method, symmetry, avoiding order reduction in time

1. Introduction

Exponential methods have been proved to be efficient in the numerical time integration of partial differential equations [16] although some times they show order reduction [4, 14]. Moreover, they have been usually used when considering homogeneous boundary conditions and the analysis has been performed under that assumption. Just some recent research [5, 6, 13] has been done to include non-homogeneous boundary conditions. Moreover, the techniques which are suggested there manage to avoid order reduction for both homogeneous and non-homogeneous boundary conditions. ([5] and [6] deal with Lawson and splitting methods when integrating linear problems and [13] with splitting methods for reaction-diffusion ones.)

In this paper, we will focus on the numerical integration of the nonlinear Schrödinger equation subject to Dirichlet boundary conditions. More precisely,

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we search for the function $u \in C^1([0,T], H^2(\Omega,\mathbb{C}))$ such that

$$\begin{aligned} u_t(\mathbf{x},t) &= i(\Delta u(\mathbf{x},t) + f(|u(\mathbf{x},t)|^2)u(\mathbf{x},t)), \quad t \in [0,T], \quad \mathbf{x} \in \Omega, \\ u(\mathbf{x},0) &= u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \partial u(t) &= g(t), \end{aligned} \tag{1}$$

for a bounded domain Ω with smooth enough boundary $\partial\Omega$, where ∂ is the Dirichlet trace operator in $H^2(\Omega)$ [12], f is a smooth enough real function, $u_0 \in H^2(\Omega,\mathbb{C})$ and $g \in C^1([0,T], H^{\frac{3}{2}}(\partial\Omega),\mathbb{C})$. (The precise conditions which are sufficient to assure the existence, uniqueness and well-posedness of such a solution, until a certain time $T > 0$, are non-trivial [7].) This problem has applications, for example, in ionospheric modification experiments [8].

For the time integration we will focus on Strang method, which is a symmetric splitting method with classical order 2. The great advantage of using a splitting method for the nonlinear Schrödinger equation is that, as firstly noticed in [18], each part resulting from the decomposition

$$u_t = i\Delta u, \tag{2}$$

$$u_t = if(|u|^2)u, \tag{3}$$

can be solved as linear, which leads to a very easy and cheap implementation. This comes from the fact that the solution of (3) leaves $|u|$ invariant. (In fact, neglecting the error coming from the space discretization, both equations are exactly solvable.)

We shall offer a cheap technique to discretize (1) with Strang method in such a way that order reduction is completely avoided. The procedure is as cheap as that suggested, among other papers, in [1, 2, 3] to avoid order reduction with Runge-Kutta type methods when integrating linear problems. Notice, however, that the technique here is different because the stages are not elliptic problems any more. Moreover, for Strang method, we will suggest a slight modification of the procedure which even conserves symmetry while also avoiding order reduction.

The paper is structured as follows. Section 2 gives some preliminaries on the space discretization, Strang method and the drawbacks of dealing the problem in other different ways. Section 3 describes the technique which is suggested and gives the final formula to be implemented. In Section 4, the local error is studied with such a technique. Section 5 describes how to modify the method in order to conserve symmetry without losing order. Section 6 gives a thorough analysis of the global error of the time semidiscretization and, finally, in Section 7 some numerical experiments are shown which corroborate the previous results.

2. Preliminaries

We will assume that the spatial discretization is performed with finite-differences on a certain grid in Ω which contains some nodes in the interior and some other nodes on the boundary. More precisely, we will suppose that the discretization of the elliptic problem

$$\begin{aligned} \Delta u(\mathbf{x}) &= F(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \partial u &= g, \end{aligned}$$

where $F \in L^2(\Omega, \mathbb{C})$ and $g \in H^{\frac{3}{2}}(\Omega, \mathbb{C})$, is done by solving the following system

$$A_{h,0} R_h u + C_h g = P_h F, \tag{4}$$

where P_h is just the nodal projection on the interior grid nodes, $R_h u$ is the approximation to the values of u in them, $A_{h,0}$ is an invertible matrix which defines the discretization of the Laplacian with vanishing boundary conditions and $C_h g$ is a vector which contains information on the values of g in the boundary grid nodes. We will consider the following hypotheses:

(H1) For a certain constant M, which is independent of h, and the discrete L^2-norm, the matrices $A_{h,0}$ satisfy

$$||e^{itA_{h,0}}||_{L^2_h(\Omega)} \le M, \quad t \in [0, T].$$

(H2) There exists a subspace Z of $L^2(\Omega)$, such that, for $u \in Z$,
- (a) $\Delta_0^{-1} u \in Z$, where $\Delta_0 = \Delta|_{H^2(\Omega) \cap H^1_0(\Omega)}$.
- (b) for some ε_h which is small with h,

$$\|A_{h,0}(P_h - R_h)u\|_{L^2_h(\Omega)} \le \varepsilon_h \|u\|_Z. \tag{5}$$

(That is, when $u \in Z$, this hypothesis means that, by doing (4), a consistent approximation of the Laplacian at the interior grid nodes is achieved.)

When the boundary conditions are homogeneous ($g = 0$), a space discretization of (1) leads to a system like

$$\begin{aligned} U_h' &= i(A_{h,0} U_h + f(|U_h|.^2).U_h), \\ U_h(0) &= P_h u_0, \end{aligned} \tag{6}$$

where . denotes pointwise vectorial multiplication. In this case of vanishing boundary conditions, no order reduction of the splitting method turns up. That can be observed in the numerical experiments and will also be shown in the subsequent analysis. (In fact, numerical results in [10] also confirm that when using a pseudospectral space discretization.) More precisely, when applying Strang method to (6), the following scheme turns up

$$U_h^{n+1} = e^{\frac{k}{2} i D_{2,n}} e^{k i A_{h,0}} e^{\frac{k}{2} i D_{1,n}} U_h^n, \tag{7}$$

where U_h^n approximates $u(\cdot, t_n)$ for $t_n = nk$, with k the time stepsize,

$$D_{1,n} = \text{diag}(f(|U_h^n|.^2)), \quad D_{2,n} = \text{diag}(f(|W_h^n|.^2)), \quad W_h^n = e^{k i A_{h,0}} e^{\frac{k}{2} i D_{1,n}} U_h^n.$$

However, when considering non-homogeneous boundary conditions, the two possibilities which in principle turn up have serious drawbacks:

(i) If we first integrate (1) in space and then in time, a differential system like this turns up

$$U_h'(t) = iA_{h,0}U_h(t) + iC_h g(t) + if(|U_h|.^2).U_h, \tag{8}$$

As we will describe in an example in Section 7, $C_h g(t)$ grows when h diminishes. As Strang method applied to

$$U' = A_1 U + A_2 U + F(t)$$

leads to

$$U^{n+1} = e^{\frac{k}{2}A_1} e^{\frac{k}{2}A_2} (e^{\frac{k}{2}A_2} e^{\frac{k}{2}A_1} U^n + kF(t_n + \frac{k}{2})),$$

when integrating (8),

$$U_h^{n+1} = e^{\frac{k}{2}iD_{2,n}} e^{\frac{k}{2}iA_{h,0}} (e^{\frac{k}{2}iA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n + ikC_h g(t_n + \frac{k}{2})),$$

where

$$D_{1,n} = \text{diag}(f(|U_h^n|.^2)),$$
$$D_{2,n} = \text{diag}(f(|W_h^n|.^2)), \ W_h^n = e^{\frac{k}{2}iA_{h,0}} (e^{\frac{k}{2}iA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n + ikC_h g(t_n + \frac{k}{2})).$$

As we will see in Section 7, this leads to very poor results. The reason for that is that $C_h g$ take very big values when $h \to 0$.

(ii) Another possibility which has been used in the literature for Runge-Kutta methods on linear problems [9] and splitting methods in diffusion-reaction problems [13] is to consider the solution of

$$\begin{aligned} \Delta z(\mathbf{x}, t) &= 0, \quad \mathbf{x} \in \Omega, \\ \partial z(t) &= g(t), \end{aligned} \tag{9}$$

which is usually denoted as $K_\Delta(0)g(t)$. Then, making the difference with (1), the following initial boundary value problem with homogeneous boundary conditions turns up for $w = u - z$:

$$\begin{aligned} w_t &= i\Delta w - z_t + if(|w+z|^2)(w+z), \\ w(\mathbf{x}, 0) &= u_0(\mathbf{x}) - z(\mathbf{x}, 0), \quad \mathbf{x} \in \Omega, \\ \partial w(t) &= 0. \end{aligned}$$

When decomposing the equation as

$$w_t = i\Delta w + if(|z|^2)z - z_t, \tag{10}$$
$$w_t = if(|w+z|^2)(w+z) - if(|z|^2)z, \tag{11}$$

the corresponding splitting would probably not show order reduction according to arguments similar to those in [13]. However, this procedure has the following drawbacks: On the one hand, at each step, the calculation of z through (9) is necessary. In the one-dimensional case, that just corresponds to a straight line and can be calculated analytically, as well as z_t. However, in more dimensions, that would mean to solve two elliptic problems at each step (one for z and another for z_t with boundary g_t) when the boundary conditions and their derivatives depend on time. On the other hand, the linear part (10) is not as directly solvable as (2) because a source term turns up now and what is more serious, $|w+z|^2$ is not an invariant of (11) and therefore, that equation cannot be solved as if it were linear. Therefore, to integrate each of those parts, an additional time integrator would have to be used.

In the description and analysis of the procedure which is suggested here to avoid order reduction, we will use $\varphi_1(it\Delta_0)$, $\varphi_2(it\Delta_0)$ and $\varphi_3(it\Delta_0)$, where $\{\varphi_j\}$ are the standard functions which are used in exponential methods [16] and which are defined by

$$\varphi_j(tA) = \frac{1}{t^j}\int_0^t e^{(t-\tau)A}\frac{\tau^{j-1}}{(j-1)!}d\tau, \quad j \geq 1. \tag{12}$$

Besides, the following is well-known to be satisfied [16]:

$$\varphi_1(z) = \frac{e^z - 1}{z}, \quad \varphi_2(z) = \frac{\varphi_1(z) - 1}{z}, \quad \varphi_3(z) = \frac{\varphi_2(z) - \frac{1}{2}}{z}. \tag{13}$$

These functions are bounded in the imaginary axis, which is the place where the eigenvalues of $it\Delta_0$ lay, because Δ_0 is a selfadjoint operator in $L^2(\Omega)$. Therefore, $e^{it\Delta_0}$, $\varphi_1(it\Delta_0)$, $\varphi_2(it\Delta_0)$ and $\varphi_3(it\Delta_0)$ are operators which are bounded in L^2-norm for real t.

3. Description of the technique

In this section, we describe how to apply directly Strang exponential method to nonlinear Schrödinger equation with nonhomogeneous and possibly time-dependent Dirichlet boundary conditions in such a way that no order reduction is shown. The main idea is to integrate (1) firstly in time with suitable boundary values for the evolutionary partial differential equation and just then, to apply the space discretization to the problems that turn up.

3.1. Time semidiscretization

Starting from the numerical approximation u^n at time t_n, for the time integration of (1), we firstly tackle the nonlinear part of the problem (3) and then solve

$$\begin{aligned} v_n'(s) &= if(|u^n|^2)v_n(s), \\ v_n(0) &= u^n, \end{aligned} \tag{14}$$

considering its value at $s = k/2$. Secondly, in order to integrate the linear part (2), apart from an initial condition, we must also suggest a boundary. As we take as initial condition for this problem $v_n(\frac{k}{2})$, for the boundary we consider the first-order Taylor expansion at $s = 0$ of the searched function w_n satisfying (2). More precisely,

$$w_n(0) + s w_n'(0) = v_n(\frac{k}{2}) + s i \Delta v_n(\frac{k}{2}). \tag{15}$$

On the other hand, in order to approximate this from the data which are given in the original problem (1), we will consider the following approximation for $v_n(\frac{k}{2})$, which comes from (14),

$$v_n(\frac{k}{2}) \approx u(t_n) + \frac{k}{2} i f(|u(t_n)|^2) u(t_n). \tag{16}$$

Neglecting then terms of second order in k and s, when $u \in H^4(\Omega)$ and $f(|u|^2)u \in H^2(\Omega)$, we consider the solution of

$$\begin{aligned} w_n'(\mathbf{x}, s) &= i\Delta w_n(\mathbf{x}, s), \quad \mathbf{x} \in \Omega, \\ w_n(\mathbf{x}, 0) &= v_n(\mathbf{x}, \frac{k}{2}), \quad \mathbf{x} \in \Omega, \\ \partial w_n(s) &= \partial[u(t_n) + \frac{k}{2} i f(|u(t_n)|^2) u(t_n) + s i \Delta u(t_n)], \\ &= g(t_n) + \frac{k}{2} i f(|g(t_n)|^2) g(t_n) + s[g_t(t_n) - i f(|g(t_n)|^2) g(t_n)]. \end{aligned} \tag{17}$$

Here (17) is understood in a generalized sense, in the same way that $e^{it\Delta_0} u_0$ is understood when $\partial u_0 \neq 0$ (see [6, 17]). Notice also that the last equality just comes from (1) considering that

$$\partial[i\Delta u(t_n)] = \partial[u_t(t_n) - i f(|u(t_n)|^2) u(t_n)] = g_t(t_n) - i f(|g(t_n)|^2) g(t_n). \tag{18}$$

Finally, evaluating w_n at $s = k$ and integrating again the nonlinear part of the problem (3), we get

$$\begin{aligned} z_n'(s) &= i f(|w_n(k)|^2) z_n(s), \\ z_n(0) &= w_n(k), \end{aligned} \tag{19}$$

and then we consider

$$u^{n+1} = z_n(\frac{k}{2}). \tag{20}$$

Remark 1. *Notice that higher order terms of asymptotic expansion for the boundary of $w_n(s)$ cannot be calculated from data since*

$$v_n(\frac{k}{2}) \approx u(t_n) + \frac{k}{2} i f(|u(t_n)|^2) u(t_n) - \frac{k^2}{4} f(|u(t_n)|^2)^2 u(t_n),$$

and then,

$$w_n(0) + sw_n'(0) + \frac{s^2}{2}w_n''(0) = v_n(\frac{k}{2}) + si\Delta v_n(\frac{k}{2}) - \frac{s^2}{2}\Delta^2 v_n(\frac{k}{2})$$
$$\approx \quad u(t_n) + \frac{k}{2}if(|u(t_n)|^2)u(t_n) - \frac{k^2}{4}f(|u(t_n)|^2)^2u(t_n)$$
$$+si\Delta u(t_n) - \frac{sk}{2}\Delta(f(|u(t_n)|^2)u(t_n)) - \frac{s^2}{2}\Delta^2 u(t_n).$$

The trace of all these terms can be calculated except for $\partial\Delta(f(|u(t_n)|^2)u(t_n))$ *and* $\partial\Delta^2 u(t_n)$ *at the same time. Notice that, from (18),*

$$\partial\Delta u_t(t_n) = -ig_{tt}(t_n) - \frac{d}{dt}[f(|g(t)|^2)g(t)]|_{t=t_n},$$

and from (1),

$$\partial\Delta u_t(t_n) \quad = \quad i\partial\Delta^2 u(t_n) + i\partial\Delta(f(|u(t_n)|^2)u(t_n)).$$

Therefore, the sum of both terms can be calculated but not both of them separately.

3.2. Final formula after space discretization

When the space discretization is applied to (14),(17),(19), the following systems turn up:

$$\begin{aligned}
&V_{h,n}'(s) = i\text{diag}(f(|U_h^n|.^2)V_{h,n}(s),\\
&V_{h,n}(0) = U_h^n,\\
&W_{h,n}'(s) = iA_{h,0}W_{h,n}(s) + iC_h[g(t_n) + i\frac{k}{2}f(|g(t_n)|^2)g(t_n))\\
&\qquad\qquad +s[g_t(t_n) - if(|g(t_n)|^2)g(t_n)]], \qquad (21)\\
&W_{h,n}(0) = V_{h,n}(\frac{k}{2}),\\
&Z_{h,n}'(s) = i\text{diag}(f(|W_{h,n}(k)|.^2)Z_{h,n}(s),\\
&Z_{h,n}(0) = W_{h,n}(k).
\end{aligned}$$

Notice that the solution of (21) at $s = k$ is

$$W_{h,n}(k) = e^{ikA_{h,0}}V_{h,n}(\frac{k}{2})$$
$$+i\int_0^k e^{i(k-s)A_{h,0}}C_h\big[g(t_n) + i\frac{k}{2}f(|g(t_n)|^2)g(t_n)) + s[g_t(t_n) - if(|g(t_n)|^2)g(t_n)]\big]ds.$$

Therefore, the final formula for the implementation is the following. Starting from $U_h^0 = P_h u_0$ and denoting $\hat{V}_h^n = V_{h,n}(\frac{k}{2})$, $\hat{W}_h^n = W_{h,n}(k)$ and $U_h^{n+1} = \hat{Z}_h^n =$

$Z_{h,n}(\frac{k}{2})$, from each U_h^n we calculate U_h^{n+1} in the following way:

$$\begin{aligned}
\hat{V}_h^n &= e^{i\frac{k}{2}\mathrm{diag}(f(|U_h^n|.^2))}U_h^n, \\
\hat{W}_h^n &= e^{ikA_{h,0}}\hat{V}_h^n + ik\varphi_1(ikA_{h,0})C_h[g(t_n) + i\frac{k}{2}f(|g(t_n)|^2)g(t_n)] \\
&\quad +ik^2\varphi_2(ikA_{h,0})C_h[g_t(t_n) - if(|g(t_n)|^2)g(t_n)], \\
U_h^{n+1} &= e^{i\frac{k}{2}\mathrm{diag}(f(|\hat{W}_h^n|.^2))}\hat{W}_h^n.
\end{aligned} \tag{22}$$

Remark 2. *Notice that the information on the boundary for the numerical integration of (1) enters at each step through multiplication by matrices* $\varphi_1(ikA_{h,0})$ *and* $\varphi_2(ikA_{h,0})$*. Although one could think that the computational cost of calculating each of those terms is similar to that of calculating* $e^{ikA_{h,0}}\hat{V}_h^n$*, in practice that is not the case for finite differences. In such a case, the vector* $C_h[\cdot]$ *has many vanishing components and therefore just some columns of* $\varphi_1(ikA_{h,0})$ *and* $\varphi_2(ikA_{h,0})$ *are in fact necessary, which are of the order of the number of grid nodes on the boundary,* $O(N^{d-1})$ *against* $O(N^d)$ *for the total number of grid nodes where* d *is the dimension of the problem and* N *the average number of grid nodes in each direction. (Look at Section 7 for a particular example in one dimension in which just two columns are necessary.) For fixed stepsize* k*, once those columns are calculated at the very beginning, just a suitable linear combination of them must be added to the method at each step with this procedure.*

4. Local error

4.1. Local error of the time discretization

In order to study the local error, we consider the value $\overline{u}^{n+1}$ obtained in (20) starting from $u^n = u(t_n)$ in (14).

Theorem 3. *Let us assume that the solution* u *of (1) satisfies*

(i) $u \in C([0,T], H^4(\Omega))$,
(ii) $f(|u|^2)u \in C([0,T], H^2(\Omega))$
(iii) $f(|u|^2)^2 u \in C([0,T], L^2(\Omega))$.

Then, when integrating (1) with Strang method using the technique (14),(17), (19),(20), the local error $\rho_{n+1} = u(t_{n+1}) - \overline{u}_{n+1}$ *satisfies*

$$\|\rho_{n+1}\|_{L^2(\Omega)} = O(k^2).$$

Proof. Similarly to (14),(17),(19) and (20) and defining

$$w_{n,B}(s) = u(t_n) + i\frac{k}{2}f(|u(t_n)|^2)u(t_n) + is\Delta u(t_n), \tag{23}$$

we now consider the solutions of the following problems

$$\begin{aligned}
&\overline{v}_n'(s) = if(|u(t_n)|^2)\overline{v}_n(s), \quad \overline{v}_n(0) = u(t_n),\\
&\overline{w}_n'(s) = i\Delta\overline{w}_n(s), \quad \overline{w}_n(0) = \overline{v}_n(\frac{k}{2}), \quad \partial\overline{w}_n(s) = \partial w_{n,B}(s), \qquad (24)\\
&\overline{z}_n'(s) = if(|\overline{w}_n(k)|^2)\overline{z}_n(s), \quad \overline{z}_n(0) = \overline{w}_n(k),
\end{aligned}$$

Then, $\overline{u}^{n+1} = \overline{z}_n(\frac{k}{2})$. Notice that

$$\overline{v}_n(\frac{k}{2}) = e^{i\frac{k}{2}f(|u(t_n)|^2)}u(t_n) = u(t_n) + i\frac{k}{2}f(|u(t_n)|^2)u(t_n) + O(k^2), \qquad (25)$$

where the residue is bounded in L^2-norm because of hypothesis (iii). Then, for the difference $\overline{w}_n(s) - w_{n,B}(s)$, we have the following:

$$\begin{aligned}
\overline{w}_n'(s) - w_{n,B}'(s) &= i\Delta\overline{w}_n(s) - i\Delta u(t_n)\\
&= i\Delta(\overline{w}_n(s) - w_{n,B}(s)) + i\Delta(w_{n,B}(s) - u(t_n))\\
&= i\Delta(\overline{w}_n(s) - w_{n,B}(s)) - \frac{k}{2}\Delta(f(|u(t_n)|^2)u(t_n) - s\Delta^2 u(t_n),\\
\overline{w}_n(0) - w_{n,B}(0) &= e^{i\frac{k}{2}f(|u(t_n)|^2)}u(t_n) - u(t_n) - i\frac{k}{2}f(|u(t_n)|^2)u(t_n),\\
\partial(\overline{w}(s) - w_{n,B}(s)) &= 0.
\end{aligned}$$

Then, through a variation-of-constants formula,

$$\begin{aligned}
\overline{w}_n(s) - w_{n,B}(s) &= e^{is\Delta_0}[e^{i\frac{k}{2}f(|u(t_n)|^2)}u(t_n) - u(t_n) - i\frac{k}{2}f(|u(t_n)|^2)u(t_n)]\\
&\quad -\frac{sk}{2}\varphi_1(is\Delta_0)\Delta(f(|u(t_n)|^2)u(t_n)) - s^2\varphi_2(is\Delta_0)\Delta^2 u(t_n) = O(k^2). \qquad (26)
\end{aligned}$$

Because of the boundedness of $e^{ik\Delta_0}, \varphi_1(ik\Delta_0)$ and $\varphi_2(ik\Delta_0)$ and assumptions (i) and (ii), this implies that

$$\overline{w}_n(k) = u(t_n) + \frac{k}{2}if(|u(t_n)|^2)u(t_n) + ki\Delta u(t_n) + O(k^2),$$

which means that

$$\begin{aligned}
\overline{u}^{n+1} &= \overline{z}_n(\frac{k}{2}) = e^{i\frac{k}{2}f(|\overline{w}_n(k)|^2)}\overline{w}_n(k)\\
&= u(t_n) + kif(|u(t_n)|^2)u(t_n) + ki\Delta u(t_n) + O(k^2) = u(t_{n+1}) + O(k^2).
\end{aligned}$$

□

4.2. Local error of the full discretization

In order to define the local error after full discretization, we consider

$$\overline{U}_{h,n+1} = \overline{Z}_{h,n}(\frac{k}{2}) = e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))}\overline{W}_{h,n}(k), \qquad (27)$$

where $\overline{W}_{h,n}(s)$ solves

$$\begin{aligned}\overline{W}'_{h,n}(s) &= iA_{h,0}\overline{W}_{h,n}(s)\\ &\quad +iC_h[g(t_n)+i\frac{k}{2}f(|g(t_n)|^2)g(t_n)) + s[g_t(t_n) - if(|g(t_n)|^2)g(t_n)]],\\ \overline{W}_{h,n}(0) &= \overline{V}_{h,n}(\frac{k}{2}) = e^{i\frac{k}{2}\mathrm{diag}(f(|P_h u(t_n)|.^2)}P_h u(t_n). \end{aligned} \tag{28}$$

Then,

$$\begin{aligned}\overline{W}_{h,n}(k) &= e^{ikA_{h,0}}e^{i\frac{k}{2}\mathrm{diag}(f(|P_h u(t_n)|.^2))}P_h u(t_n)\\ &+i\int_0^k e^{i(k-s)A_{h,0}}C_h\big[g(t_n)+i\frac{k}{2}f(|g(t_n)|^2)g(t_n)) + s[g_t(t_n) - if(|g(t_n)|^2)g(t_n)]\big]ds,\end{aligned}$$

which can be inserted in (27).

We now define the local error at $t = t_n$ as

$$\rho_{h,n} = P_h u(t_n) - \overline{U}_{h,n},$$

and study its behaviour in the following theorem.

Theorem 4. *Under the same hypotheses of Theorem 3, assuming also that f is locally Lipschitz continuous, that*

$$u, f(|u|^2)u, \Delta u \in C([0,T], Z), \tag{29}$$

for the space Z which is defined in (H2) and hypotheses (H1)-(H2) for the space discretization, when integrating (1) with Strang method as described in (22),

$$\|\rho_{h,n+1}\|_{L_h^2(\Omega)} = O(k^2 + k\varepsilon_h), \tag{30}$$

where ε_h is that in (5).

Proof. Notice that

$$\rho_{h,n+1} = P_h u(t_{n+1}) - \overline{U}_{h,n+1} = P_h \rho_{n+1} + (P_h \overline{u}_{n+1} - \overline{U}_{h,n+1}).$$

Then, from Theorem 3, the first term is $O(k^2)$. In order to bound the second term, we take into account that

$$\begin{aligned}P_h\overline{u}_{n+1} - \overline{U}_{h,n+1} &= P_h\overline{z}_n(\frac{k}{2}) - \overline{Z}_{h,n}(\frac{k}{2})\\ &= P_h\big[e^{i\frac{k}{2}f(|\overline{w}_n(k)|^2)}\overline{w}_n(k)\big] - e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))}\overline{W}_{h,n}(k)\\ &= e^{i\frac{k}{2}\mathrm{diag}(P_h f(|\overline{w}_n(k)|^2))}P_h\overline{w}_n(k) - e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))}\overline{W}_{h,n}(k)\\ &= \big[e^{i\frac{k}{2}\mathrm{diag}(P_h f(|\overline{w}_n(k)|^2))} - e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))}\big]P_h\overline{w}_n(k)\\ &\qquad + e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))}[P_h\overline{w}_n(k) - \overline{W}_{h,n}(k)]. \end{aligned} \tag{31}$$

Then, considering (23),(25) and (4),

$$\begin{aligned}
P_h w'_{n,B}(s) &= iP_h\Delta u(t_n) \\
&= i[P_h\Delta w_{n,B}(s) - i\frac{k}{2}P_h\Delta(f(|u(t_n)|^2)u(t_n)) - isP_h\Delta^2 u(t_n)] \\
&= iA_{h,0}R_h w_{n,B}(s) + iC_h\partial w_{n,B}(s) + \frac{k}{2}P_h\Delta(f(|u(t_n)|^2)u(t_n)) \\
&\quad + sP_h\Delta^2 u(t_n) \\
&= iA_{h,0}P_h w_{n,B}(s) + iC_h\partial w_{n,B}(s) + iA_{h,0}(R_h - P_h)w_{n,B}(s) \\
&\quad + \frac{k}{2}P_h\Delta(f(|u(t_n)|^2)u(t_n)) + sP_h\Delta^2 u(t_n) \\
P_h w_{n,B}(0) &= P_h u(t_n) + i\frac{k}{2}f(|P_h u(t_n)|.^2).P_h u(t_n). \qquad (32)
\end{aligned}$$

Making now the difference with (28), we have that

$$\begin{aligned}
P_h w'_{n,B}(s) - \overline{W}'_{h,n}(s) &= iA_{h,0}[P_h w_{n,B}(s) - \overline{W}_{h,n}(s)] + iA_{h,0}(R_h - P_h)w_{n,B}(s) \\
&\quad + \frac{k}{2}P_h\Delta(f(|u(t_n)|^2)u(t_n)) + sP_h\Delta^2 u(t_n), \\
P_h w_{n,B}(0) - \overline{W}_{h,n}(0) &= P_h u(t_n) + i\frac{k}{2}f(|P_h u(t_n)|.^2).P_h u(t_n) \\
&\quad - e^{i\frac{k}{2}\mathrm{diag}(f(|P_h u(t_n)|.^2))}P_h u(t_n),
\end{aligned}$$

which implies that

$$\begin{aligned}
P_h w_{n,B}(k) - \overline{W}_{h,n}(k) = e^{ikA_{h,0}}O(k^2) + i\int_0^k e^{i(k-s)A_{h,0}}A_{h,0}(R_h - P_h)w_{n,B}(s)ds \\
+ \int_0^k e^{i(k-s)A_{h,0}}[\frac{k}{2}P_h\Delta(f(|u(t_n)|^2)u(t_n)) + sP_h\Delta^2 u(t_n)] = O(k\epsilon_h + k^2).
\end{aligned}$$

The last equality is deduced from (H1) and (5) using also that $w_{n,B}(s) \in Z$ because of (23) and (29). Now, from (26), it is straightforward that

$$P_h\overline{w}_n(k) - \overline{W}_{h,n}(k) = O(k\epsilon_h + k^2). \qquad (33)$$

On the other hand, by considering the component-wise Taylor expansion of the exponential,

$$\begin{aligned}
&e^{i\frac{k}{2}\mathrm{diag}(P_h f(|\overline{w}_n(k)|^2))} - e^{i\frac{k}{2}\mathrm{diag}(f(|\overline{W}_{h,n}(k)|.^2))} \\
&\quad = i\frac{k}{2}[P_h f(|\overline{w}_n(k)|^2) - f(|\overline{W}_{h,n}(k)|.^2)] + O(k^2) = O(k^2(\epsilon_h + 1)),
\end{aligned}$$

where we have used (33), the fact that f is locally Lipschitz continuous and that $\overline{w}_n(k)$ is bounded because of (26). Inserting this together with (33) in (31), the result follows. □

5. How to conserve symmetry when avoiding order reduction

Splitting exponential methods integrating nonlinear Schrödinger equation have the big advantage of integrating the linear and nonlinear part of the equation in an exact way, except for the error coming from the space discretization or from the boundaries which are implicitly imposed when integrating the linear part. Apart from that, Strang method has the additional attractive feature of being in principle a symmetric method and therefore conserving the time-reversibility of the equation. The technique to avoid order reduction which is described in the previous section implies to lose that symmetry because the boundary for w_n which is suggested in (17) is based on an asymptotic expansion of $v_n(\frac{k}{2})$ at $s = 0$ and therefore depends on values of the boundary of the solution at t_n. If we want to preserve symmetry, when integrating backwards from t_{n+1}, that boundary should be the same. In this section, we will see how to conserve that symmetry when avoiding order reduction and moreover, independently of the space discretization being used for the Laplacian.

When integrating regular enough solutions of ordinary differential systems, symmetry implies that the local error behaves as $O(k^{p+1})$ with even p [15]. Unfortunately, this is not the case here and therefore we will not be able to increase the order of the local error by conserving symmetry. The reason which makes that the argument for ODEs cannot be applied here is that we do not have an asymptotic expansion of the local error with a term in k^2 and another one in k^3. (In the proof of Theorem 3 we had to stop at k^2 because of the unboundedness of the operator Δ_0.)

5.1. Modification of the technique and proof of symmetry

Instead of approximating $v_n(\frac{k}{2})$ as in (16), we can consider

$$v_n(\frac{k}{2}) \approx u(t_{n+\frac{1}{2}}) - \frac{k}{2} i\Delta u(t_{n+\frac{1}{2}}),$$

which just differs from (16) in $O(k^2)$ because of (1). Then, substituting this expression in (15) and neglecting terms of second order in k and s, we suggest the following for the boundary of w_n, which can again be calculated in terms of data because of (18):

$$\begin{aligned} \partial w_n(s) &= \partial u(t_{n+\frac{1}{2}}) + (s - \frac{k}{2}) i\partial\Delta u(t_{n+\frac{1}{2}}) \\ &= g(t_{n+\frac{1}{2}}) + (s - \frac{k}{2})[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]. \end{aligned} \quad (34)$$

Inserting this in (17) and applying afterwards the space discretization, the following formula is obtained for $\hat{W}_h^n$, which is the only one which must be changed in (22):

$$\begin{aligned} \hat{W}_h^n = e^{ikA_{h,0}}\hat{V}_h^n + ik\varphi_1(ikA_{h,0})C_h\big[g(t_{n+\frac{1}{2}}) \\ -\frac{k}{2}[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]\big] \\ +ik^2\varphi_2(ikA_{h,0})C_h[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]. \end{aligned} \quad (35)$$

The following theorem states the symmetry for the time semidiscretization.

Theorem 5. *The procedure given by (14), (17) with boundary (34), (19) and (20) to integrate (1) with Strang method is symmetric.*

Proof. It suffices to see that, starting from u^{n+1} and advancing with stepsize $-k$ with the same procedure, we arrive at u^n. For that, notice that $u^{n+1} = e^{i\frac{k}{2}f(|w_n(k)|^2)}w_n(k)$ and therefore $|u^{n+1}| = |w_n(k)|$. Now, for the backwards integration we will use tilde notation and, in a similar way to (14), we have

$$\begin{aligned} \tilde{v}'_{n+1}(s) &= if(|u^{n+1}|^2)\tilde{v}_{n+1}(s), \\ \tilde{v}_{n+1}(0) &= u^{n+1}. \end{aligned}$$

Therefore, $\tilde{v}_{n+1}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|u^{n+1}|^2)}e^{i\frac{k}{2}f(|w_n(k)|^2)}w_n(k) = w_n(k)$. Then, the equivalent of (17) with boundary (34) changing k by $-k$ and starting from the latter function is

$$\begin{aligned} \tilde{w}'_{n+1}(s) &= i\Delta\tilde{w}_{n+1}(s), \\ \tilde{w}_{n+1}(0) &= w_n(k), \\ \partial\tilde{w}_{n+1}(s) &= g(t_{n+\frac{1}{2}}) + (s+\frac{k}{2})[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]. \end{aligned}$$

It is direct to see that $\tilde{w}_{n+1}(s) = w_n(s+k)$ because both functions satisfy the same equation, have the same value at $s=0$ and have the same boundary. As a consequence, $\tilde{w}_{n+1}(-k) = w_n(0) = v_n(\frac{k}{2})$. Taking this into account, the equivalent to (19) would be

$$\begin{aligned} \tilde{z}'_{n+1}(s) &= if(|v_n(\frac{k}{2})|^2)\tilde{z}_{n+1}(s), \\ \tilde{z}_{n+1}(0) &= v_n(\frac{k}{2}), \end{aligned}$$

and therefore $\tilde{z}_{n+1}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|v_n(\frac{k}{2})|^2)}v_n(\frac{k}{2})$. As $v_n(\frac{k}{2}) = e^{i\frac{k}{2}f(|u^n|^2)}u^n$ and then $|v_n(\frac{k}{2})| = |u^n|$, it follows that $\tilde{z}_{n+1}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|u^n|^2)}e^{i\frac{k}{2}f(|u^n|^2)}u^n = u^n$, which implies the result. □

The next theorem assures that the symmetry is also conserved exactly after space discretization for any diagonallizable discretization of the Laplacian with vanishing boundary conditions and any operator C_h concerning the boundary.

Theorem 6. *Whenever $A_{h,0}$ is diagonallizable, the procedure given by (22) with $\hat{W}_h^n$ substituted by (35) to integrate (1) with Strang method is symmetric.*

Proof. As in the previous theorem, we will see that starting from U_h^{n+1} and advancing with stepsize $-k$, we arrive at U_h^n. As $U_h^{n+1} = e^{i\frac{k}{2}\mathrm{diag}(|f(\hat{W}_h^n)|.^2)}\hat{W}_h^n$, going backwards

$$\tilde{\tilde{V}}_h = e^{-i\frac{k}{2}\mathrm{diag}(f(|U_h^{n+1}|.^2))}e^{i\frac{k}{2}\mathrm{diag}(f(|\hat{W}_h^n|.^2))}\hat{W}_h^n = \hat{W}_h^n.$$

Then, considering this in (35) with k substituted by $-k$,

$$\begin{aligned}
\tilde{\hat{W}}_h^{n+1} &= e^{-ikA_{h,0}}\hat{W}_h^n - ik\varphi_1(-ikA_{h,0})C_h\big[g(t_{n+\frac{1}{2}}) + \frac{k}{2}[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]\big] \\
&\quad + ik^2\varphi_2(-ikA_{h,0})C_h[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})].
\end{aligned}$$

Substituting then here $\hat{W}_h^n$ by the forward expression (35),

$$\begin{aligned}
\tilde{\hat{W}}_h^{n+1} &= e^{-ikA_{h,0}}\Big[e^{ikA_{h,0}}\hat{V}_h^n + ik\varphi_1(ikA_{h,0})C_h\big[g(t_{n+\frac{1}{2}}) - \frac{k}{2}[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]\big] \\
&\qquad + ik^2\varphi_2(ikA_{h,0})C_h[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]\Big] \\
&\quad - ik\varphi_1(-ikA_{h,0})C_h\big[g(t_{n+\frac{1}{2}}) + \frac{k}{2}[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]\big] \\
&\quad + ik^2\varphi_2(-ikA_{h,0})C_h[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})]. \\
&= \hat{V}_h + ik[e^{-ikA_{h,0}}\varphi_1(ikA_{h,0}) - \varphi_1(-ikA_{h,0})]C_h g(t_{n+\frac{1}{2}}) \\
&\quad + ik^2\big[-\frac{1}{2}(e^{-ikA_{h,0}}\varphi_1(ikA_{h,0}) + \varphi_1(-ikA_{h,0})) \\
&\qquad + e^{-ikA_{h,0}}\varphi_2(ikA_{h,0}) + \varphi_2(-ikA_{h,0})\big]C_h[g_t(t_{n+\frac{1}{2}}) - if(|g(t_{n+\frac{1}{2}})|^2)g(t_{n+\frac{1}{2}})].
\end{aligned}$$

Now, notice that the coefficients of k and k^2 vanish when $A_{h,0}$ is diagonallizable since, because of (13),

$$\begin{aligned}
& e^{-z}\varphi_1(z) - \varphi_1(-z) = 0, \\
& -\frac{1}{2}(e^{-z}\varphi_1(z) + \varphi_1(-z)) + e^{-z}\varphi_2(z) + \varphi_2(-z) \\
&\qquad\qquad = -\varphi_1(-z) + \frac{\varphi_1(-z) - e^{-z}}{z} - \frac{\varphi_1(-z) - 1}{z} = 0.
\end{aligned}$$

Therefore, $\tilde{\hat{W}}_h^{n+1} = \hat{V}_h^n$ and considering that $\hat{V}_h^n = e^{i\frac{k}{2}\mathrm{diag}(f(|U_h^n|.^2))}U_h^n$,

$$\tilde{\hat{Z}}_h^{n+1} = e^{-i\frac{k}{2}\mathrm{diag}(f(|\tilde{\hat{W}}_h^{n+1}|.^2))}\tilde{\hat{W}}_h^{n+1} = e^{-i\frac{k}{2}\mathrm{diag}(f(|\hat{V}_h^n|.^2))}\hat{V}_h^n = U_h^n.$$

□

5.2. Local error

In a similar way to Theorem 3, we do have the following result:

Theorem 7. *Let us assume that f in (1) is a continously differentiable function and that the solution u of that problem satisfies, apart from hypotheses (i),(ii) and (iii) in Theorem 3,*

(iv) $f'(|u|^2)u^2\Delta u \in C([0,T], L^2(\Omega))$,
(v) $f(|u|^2)\Delta u \in C([0,T], L^2(\Omega))$.

Then, when integrating (1) with Strang method using the procedure (14), (17) with boundary (34), (19) and (20), the local error $\rho_{n+1} = u(t_{n+1}) - \overline{u}_{n+1}$ satisfies

$$\|\rho_{n+1}\|_{L^2(\Omega)} = O(k^2).$$

Proof. This is proved in the same way as Theorem 3 with the difference that now the boundary for $\overline{w}_n(s)$ is given by

$$w_{n,SB}(s) = u(t_{n+\frac{1}{2}}) + (s - \frac{k}{2}) i\Delta u(t_{n+\frac{1}{2}}),$$

and

$$\overline{w}_n(0) - w_{n,SB}(0) = e^{i\frac{k}{2} f(|u(t_n)|^2)} u(t_n) - u(t_{n+\frac{1}{2}}) + \frac{k}{2} i\Delta u(t_{n+\frac{1}{2}}).$$

By considering asymptotic expansions on k around $u(t_n)$, this expression can be calculated to be $O(k^2)$ in the L^2-norm because of assumptions (i)-(v). □

From here, with the same proof as that of Theorem 4, the following result follows.

Theorem 8. *Under the same hypotheses of Theorem 7 and assuming also (29) for the space Z which is defined in (H2) and hypotheses (H1)-(H2) for the space discretization, when integrating (1) with Strang method as described in (22) with $\hat{W}_h^n$ substituted by (35),*

$$\|\rho_{h,n+1}\|_{L_h^2(\Omega)} = O(k^2 + k\varepsilon_h),$$

where ε_h is that in (5).

6. Global error

For the sake of brevity, we will focus here on the global error coming from the time semidiscretization, which is the main aim of the paper. We will see that, although classically local order 2 leads to global order 1, under assumptions of regularity a summation-by-parts argument applies and global order is also 2.

Theorem 9. *Under hypotheses of Theorem 3 (resp. 7), assuming also that*

$$f(|u|^2)u \in C^1([0,T], H^4(\Omega)), u \in C^1([0,T], H^6(\Omega)), \tag{36}$$

and that the following functions are well defined in $C^1([0,T], L^2(\Omega))$:

$$f(|u|^2)^3 u, f(|u|^2)\Delta(f(|u|^2 u), f(|u|^2)\Delta^2 u, f'(|u|^2)u^2\Delta(f(|u|^2)u), f'(|u|^2)u^2\Delta^2 u,$$
$$f'(|u|^2)f(|u|^2)u^2\Delta u, f'(|u|^2)u|\Delta u|^2, f(|u|^2)u^2\Delta u, (\Delta u)^2 u, f(|u|^2)\Delta u, u_{ttt}, \tag{37}$$

applying the technique which is stated in the above theorems, it happens that

$$\|e_n\|_{L^2(\Omega)} = O(k^2).$$

Proof. Firstly, notice that, as f is continuously differentiable, if $u_1, u_2 \in L^2(\Omega)$,

$$e^{i\frac{k}{2}f(|u_1|^2)}u_1 - e^{i\frac{k}{2}f(|u_2|^2)}u_2 = (u_1 - u_2) + \frac{k}{2}E(u_1, u_2),$$

where, for some constant C,

$$\|E(u_1, u_2)\|_{L^2(\Omega)} \leq C\|u_1 - u_2\|_{L^2(\Omega)}.$$

Considering the notation $e_n = u(t_n) - u^n$ for the global error, the standard argument to relate it to local error gives:

$$\begin{aligned} e_{n+1} &= u(t_{n+1}) - u^{n+1} = (u(t_{n+1}) - \overline{u}^{n+1}) + (\overline{u}^{n+1} - u^{n+1}) \\ &= \rho_{n+1} + \left[e^{i\frac{k}{2}f(|\overline{w}_n(k)|^2)}\overline{w}_n(k) - e^{i\frac{k}{2}f(|w_n(k)|^2)}w_n(k)\right] \\ &= \rho_{n+1} + \overline{w}_n(k) - w_n(k) + \frac{k}{2}E(\overline{w}_n(k), w_n(k)), \end{aligned} \tag{38}$$

Now, making the difference between (17) and (24),

$$\begin{aligned} &\overline{w}_n(k) - w_n(k) = e^{ik\Delta_0}(\overline{v}_n(\frac{k}{2}) - v_n(\frac{k}{2})) \\ &\quad = e^{ik\Delta_0}(e^{i\frac{k}{2}f(|u(t_n)|^2)}u(t_n) - e^{i\frac{k}{2}f(|u^n|^2)}u^n) = e^{ik\Delta_0}(e_n + \frac{k}{2}E(u(t_n), u^n)), \end{aligned}$$

which, inserted in (38), implies that

$$e_{n+1} = \rho_{n+1} + e^{ik\Delta_0}e_n + kF(u(t_n), u^n),$$

where

$$\|F(u(t_n), u^n)\|_{L^2(\Omega)} \leq C'\|e_n\|_{L^2(\Omega)}. \tag{39}$$

Applying this inductively, as $e_0 = 0$,

$$e_n = \sum_{l=1}^{n} e^{i(n-l)k\Delta_0}\rho_l + k\sum_{l=0}^{n-1} e^{i(n-l-1)k\Delta_0}F(u(t_l), u^l). \tag{40}$$

Now we use the decomposition

$$\sum_{l=1}^{n} e^{ik(n-l)\Delta_0}\rho_l = (\sum_{r=1}^{n-1} e^{irk\Delta_0})\rho_1 + \sum_{j=2}^{n-1}\big(\sum_{r=1}^{j-1} e^{irk\Delta_0}\big)(\rho_{n-j+1} - \rho_{n-j}) + \rho_n, \tag{41}$$

and we consider that, as stated in [11], for any $\eta \in H^2(\Omega) \cap H_0^1(\Omega)$,

$$\|ki\Delta_0 \sum_{r=1}^{n-1} e^{irk\Delta_0}\eta\|_{L^2(\Omega)} \leq T\|\eta\|_{H^2(\Omega)}.$$

Then, by proving that $\|\Delta_0^{-1}\rho_1\|_{H^2(\Omega)} = O(k^3)$ and $\|\Delta_0^{-1}(\rho_{n-j+1} - \rho_{n-j})\|_{H^2(\Omega)} = O(k^4)$, and inserting this in (41) and then in (40), the result follows by applying discrete Gronwall's inequality.

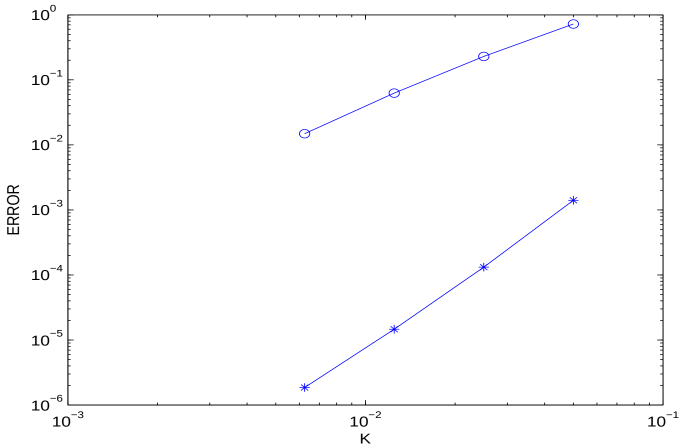

Figure 1: Local error (*) and global error (o) with vanishing boundary conditions

For the sake of brevity, we will restrict the proof of $\|\Delta_0^{-1}\rho_n\|_{H^2(\Omega)} = O(k^3)$ to the case of the assumptions of Theorem 3. Notice that, in such a case, if we allow to use unbounded operators Δ_0, by using (13), we can write $\overline{w}_n(k)$ in (26) as

$$\begin{aligned}\overline{w}_n(k) &= u(t_n) + i\frac{k}{2}f(|u(t_n)|^2)u(t_n) + ik\Delta u(t_n)\\ &\quad -(I + ik\Delta_0\varphi_1(ik\Delta_0))(\frac{k^2}{8}f(|u(t_n)|^2)^2u(t_n) + \frac{k^3}{48}f(|u(t_n)|^2)^3u(t_n) + \cdots)\\ &\quad -\frac{k^2}{2}(I + ik\Delta_0\varphi_2(ik\Delta_0))\Delta(f(|u(t_n)|^2)u(t_n))\\ &\quad -k^2(\frac{1}{2}I + ik\Delta_0\varphi_3(ik\Delta_0))\Delta^2u(t_n).\end{aligned}$$

By inserting this in

$$\Delta_0^{-1}\rho_{n+1} = \Delta_0^{-1}\big[e^{i\frac{k}{2}f(|\overline{w}_n(k)|^2)}\overline{w}_n(k) - u(t_{n+1})\big],$$

and making the corresponding asymptotic expansions on k, it can be checked that the coefficient of k^2 vanishes and that of k^3 is bounded in $H^2(\Omega)$ because of the hypotheses of regularity. Moreover, because of the same hypothesis, the expression is continously differentiable in t_n and therefore one more power of k can be obtained for the difference $\|\Delta_0^{-1}(\rho_{n-j+1} - \rho_{n-j})\|_{H^2(\Omega)}$.

□

7. Numerical experiments

In this section, we will show some numerical experiments which corroborate the previous results. For that, we will integrate the one-dimensional problem

k	0.1	5×10^{-2}	2.5×10^{-2}	1.25×10^{-2}
Local order		3.42	3.17	2.97
Global order		1.65	1.87	2.07

Table 1: Orders for the local and global error with vanishing boundary conditions

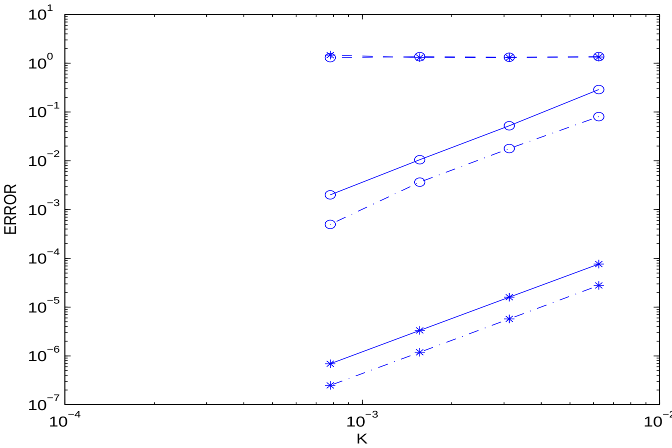

Figure 2: Local error (*) and global error (o) with non-vanishing boundary conditions, avoiding order reduction without conserving symmetry (cont. line), avoiding order reduction conserving symmetry (dash-dotted line) and not avoiding order reduction (discont. line)

k	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}	7.8125×10^{-4}
Local order		2.26	2.26	2.27
Global order		2.47	2.31	2.40

Table 2: Orders for the local and global error with non-vanishing boundary conditions using procedure (22)

(1) in $\Omega = (a, b)$ with $f(x) = 8x$ and data u_0 and g such that the solution is

$$u(x,t) = e^{it}\mathrm{sech}(x)\frac{1+\frac{3}{4}\mathrm{sech}(x)^2(e^{8it}-1)}{1-\frac{3}{4}\mathrm{sech}(x)^4\sin(4t)^2}.$$

Notice that this solution is very regular and therefore all hypotheses (i)-(v) in Theorems 3 and 7 are satisfied, as well as (29) in Theorems 4 and 8 and (36)-(37) in Theorem 9.

For the space discretization of the Laplacian we will consider the second-order symmetric difference scheme, for which

$$A_{h,0} = \frac{1}{h^2}\mathrm{tridiag}(1,-2,1), \quad C_h g(t) = \frac{1}{h^2}[g_a(t), 0, \cdots, 0, g_b(t)]^T,$$

where $g_a(t)$ and $g_b(t)$ are the Dirichlet boundary conditions at the interval end-points. As $A_{h,0}$ is symmetric and its eigenvalues are real, (H1) follows with $M = 1$ because the spectral radius of $e^{itA_{h,0}}$ is 1. Moreover, it is well-known that (5) is satisfied with $Z = H^4(a, b)$. Even more, (H2a) is satisfied because if $u \in H^4(a, b)$, $\Delta_0^{-1}u \in H^6(a, b) \subset H^4(a, b)$.

When considering $(a, b) = (-50, 50)$, the boundary conditions can be considered as homogeneous and therefore, in such a case, no order reduction is shown when integrating (1) directly through (7) with Strang method. Figure 1, which shows the local and global error against the stepsize k when integrating till time $T = 1$, corroborates that for $h = 1/64$. (This value of h makes the error in space negligible compared to that in time.) Notice that, in this case, procedure (22) is in fact the same as (7). In fact, Table 1 shows the estimated values of the orders which come from consecutive values of the error and order near 3 can be observed for the local error and near 2 for the global one. Notice that, in this case, the additional values for the boundary of $w_n(s)$ which would be required to obtain order 3 according to Remark 1, would vanish and therefore this explains that order 3 is observed for the local error.

However, when $(a, b) = (0, 1)$, the boundary conditions are not homogeneous any more. Then, applying Strang method directly to (8) as described in the preliminaries gives rise to very bad results which do not even diminish when the considered values of the time stepsizes decrease. That can be observed in Figure 2, where $h = 1/400$ has been used for the space discretization. However, when applying the technique (22) which is justified in this paper, order even a bit more than 2 is observed for the local and global errors, as Figure 2 and Table 2 shows. This corroborates Theorems 4 and 9. Moreover, if (22) is applied with $\hat{W}_h^n$ calculated through (35), the symmetry of the method is conserved and no order reduction is either shown, as it can be observed in the same figure and in Table 3. Theorem 8 and again Theorem 9 are then corroborated and the numerical results show that the approximation is more accurate.

Moreover, we remember that the cost of avoiding order reduction is negligible compared to the rest of the calculations, as it was explained in Remark 2. In that sense, we give a comparison in terms of CPU time, for this problem, when considering the technique in [13], which was explained in part (ii) of Section

k	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}	7.8125×10^{-4}
Local order		2.28	2.27	2.26
Global order		2.17	2.29	2.88

Table 3: Orders for the local and global error with non-vanishing b. c. using procedure (22) with $\hat{W}_{h}^{n}$ substituted by (35) and therefore conserving symmetry for Strang method, $h = 2.5 \times 10^{-3}$.

2. In the same way as in that paper, Crank-Nicolson has been used for the integration of (10) and the classical fourth-order Runge-Kutta method for (11). As for the methods which are suggested in this paper, we have calculated the terms of the form $e^{ikA_{h,0}}U_h$ by using the fast sine discrete transform, taking into account that the eigenvalues and eigenvectors of $A_{h,0}$ are well-known in this case and that an argument similar to a fast Poisson solver can be applied. It is clear from Figure 3 that the method in [13] also leads to global order around 2. However, the symmetric method which is suggested in this paper manages to get the same error with less computational time. In more dimensions, the comparison would be more favourable for the generalizations of Strang method which are suggested here since the calculation of z in (10)-(11) would not be so direct and would imply an additional cost.

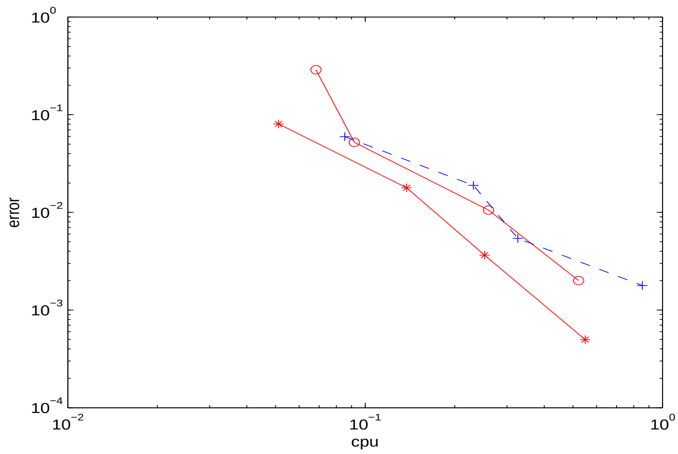

Figure 3: Error against cpu time when $h = 1/400$ and the values of k in Table 2 for the non-symmetric technique suggested here (o and continuous line), the symmetric technique suggested here (* with continuous line) and the technique suggested in [13] (+ and discontinuous line)

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