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A POSTERIORI ERROR ANALYSIS FOR THE CRANK-NICOLSON METHOD FOR LINEAR SCHRÖDINGER EQUATIONS*

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Abstract. We prove *a posteriori* error estimates of optimal order for linear Schrödinger-type equations in the $L^\infty(L^2)$- and the $L^\infty(H^1)$-norm. We discretize only in time by the Crank-Nicolson method. The direct use of the reconstruction technique, as it has been proposed by Akrivis *et al.* in [*Math. Comput.* **75** (2006) 511–531], leads to *a posteriori* upper bounds that are of optimal order in the $L^\infty(L^2)$-norm, but of suboptimal order in the $L^\infty(H^1)$-norm. The optimality in the case of $L^\infty(H^1)$-norm is recovered by using an auxiliary initial- and boundary-value problem.

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1. Introduction

In this paper we focus on the *a posteriori* error analysis for time discrete Crank-Nicolson approximations, of linear Schrödinger-type equations in the $L^\infty(L^2)$- and the $L^\infty(H^1)$-norm.

To fix notation, let $\Omega \subset \mathbb{R}^d$ be a bounded domain with boundary $\partial\Omega$ and let $0 < T < \infty$ be given. The initial- and boundary-value problem for the general linear Schrödinger equation reads as

$$\begin{cases} u_t - \mathrm{i}\alpha\Delta u + \mathrm{i}g(x,t)u = f(x,t) & \text{in } \bar{\Omega}\times[0,T], \\ u = 0 & \text{on } \partial\Omega\times[0,T], \\ u(\cdot,0) = u_0 & \text{in } \bar{\Omega}, \end{cases} \tag{1.1}$$

where α is a positive constant, $g : \bar{\Omega}\times[0,T] \to \mathbb{R}$ and $f : \bar{\Omega}\times[0,T] \to \mathbb{C}$ are given functions and $u_0 : \bar{\Omega} \to \mathbb{C}$ is a given initial value. Problem (1.1) can be equivalently written, for $t \in [0,T]$, in variational form as

$$\begin{cases} (u_t(t), \upsilon) + \mathrm{i}\alpha(\nabla u(t), \nabla\upsilon) + \mathrm{i}\big(g(t)u(t), \upsilon\big) = \big(f(t), \upsilon\big), & \forall \upsilon \in H_0^1(\Omega), \\ u(\cdot,0) = u_0 & \text{in } \bar{\Omega}, \end{cases} \tag{1.2}$$

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where $(\cdot,\cdot)$ denotes the L^2-inner product in Ω. It is well known that, if

$$\begin{cases} g \in C^1\big([0,T];C^1(\bar{\Omega})\big),\\ f \in L^2\big([0,T];L^2(\Omega)\big),\ f_t \in L^2\big([0,T];H^{-1}(\Omega)\big),\\ u_0 \in H_0^1(\Omega), \end{cases} \tag{1.3}$$

then problem (1.2) has a unique weak solution $u \in C\big([0,T];H_0^1(\Omega)\big)$; also $u_t \in C\big([0,T];\,H^{-1}(\Omega)\big)$, *cf.*, *e.g.*, [7], pp. 620–630, [1,10] and references [6,15] therein.

A posteriori error estimates for problem (1.1) (or equivalently for problem (1.2)) in the $L^\infty(L^2)$-norm for the Crank-Nicolson method have been proven by Dörfler in [8]; these estimates are of first order of accuracy in time. As a continuation of this paper, Katsaounis and Kyza prove in [11] (see also [14], Chap. 7), optimal $L^\infty(L^2)$ *a posteriori* error estimates for fully discrete schemes. The derivation of the basic estimates in [11] follows the approach in [17], *i.e.*, an appropriate reconstruction is used which involves the Crank-Nicolson reconstruction that has been proposed by Akrivis *et al.* in [2]. Another Crank-Nicolson reconstruction that has been proposed by Lozinski *et al.* in [16], has been used in [14], to obtain similar estimates.

Our aim in this paper is to provide an error control of *a posteriori* type for Crank-Nicolson time discrete approximations of linear Schrödinger equation in the $L^\infty(L^2)$- and the $L^\infty(H^1)$-norm. Estimates in the $L^\infty(H^1)$-norm are crucial in the $L^\infty(L^2)$ error analysis of the nonlinear Schrödinger equation with cubic nonlinearities (cubic NLS). In particular, to complete the arguments in this case, we must have at our disposal $L^\infty(H^1)$ error estimates, *cf.* [12,13] for the *a priori* error analysis and [14], Chapter 3, for the *a posteriori* error analysis. More precisely, regarding the *a posteriori* analysis, standard energy techniques are not enough to lead to estimates in the $L^\infty(L^2)$-norm for the two-dimensional cubic NLS. A natural approach then is to take advantage of Strichartz estimates that are valid for the Schrödinger operator, *cf.* [4]. Strichartz estimates are related to the $L^\infty(H^1)$-norm and inevitably the proof of $L^\infty(H^1)$ *a posteriori* error estimates becomes a necessity. The derivation of *a posteriori* error estimates in the $L^\infty(H^1)$-norm for the nonlinear case will be the subject of a forthcoming paper. Note, however, that having at hand such estimates in the linear case comprises an important starting point for the proof of the corresponding estimates in the nonlinear case.

To obtain the *a posteriori* error estimates in the linear case, we will use energy techniques and the Crank-Nicolson reconstruction proposed in [2]. The derivation of the $L^\infty(H^1)$-estimates in this case is more involved compared to the $L^\infty(L^2)$-estimates. The direct application of the reconstruction technique, as it is proposed in [2], leads to suboptimal $L^\infty(H^1)$ upper bounds. As we shall see in Section 4, to recover the optimality we need to use technically more involved arguments compared to [2] and new key ideas. In particular, the introduction of an auxiliary initial- and boundary-value problem will play a significant role for the analysis of Section 4.

More precisely, the paper is organized as follows: In Section 2 we introduce the Crank-Nicolson method and the reconstruction for problem (1.1). In Section 3 we discuss the regularity of the reconstruction and we address the optimal order *a posteriori* error estimate in the $L^\infty(L^2)$-norm, Theorem 3.1.

The main results of the paper are stated in Section 4. In particular, Section 4 deals with the *a posteriori* error analysis in the $L^\infty(H^1)$-norm. To prove the estimates, we first proceed as in the *a priori* error analysis for Schrödinger-type equations (see for example [12,13]), but in the continuous level instead of the discrete. From this procedure we conclude that to prove an optimal *a posteriori* error estimate in the $L^\infty(H^1)$-norm, we first need to estimate *a posteriori* the quantity $\sup_{0\le t\le T}\|\hat{e}_t(t)\|_{L^2(\Omega)}$, where $\hat{e}$ represents the error between the exact solution and the reconstruction (see Sect. 3). The "obvious way" to do this leads to suboptimal upper bounds, Theorem 4.1. In the second part of Section 4 we describe in detail how we can recover the optimality. The estimates of optimal order of accuracy for the general case are presented in Theorems 4.2 and 4.3. In the special case $f \equiv 0$ and function g is independent of the time variable, we conclude some simplifications on the main results, which are presented in the last part of Section 4. The case $f \equiv 0$ and $g \equiv g(x)$ is very interesting, since the so-called linear Schrödinger equation in the semiclassical regime,

$$u_t - \mathrm{i}\frac{\varepsilon}{2}\Delta u + \frac{\mathrm{i}}{\varepsilon}V(x)u = 0, \tag{1.4}$$

is a special case of it with $\alpha := \frac{\varepsilon}{2}$ and $g := \frac{1}{\varepsilon}V$. In (1.4), ε $(0 < \varepsilon \ll 1)$ is the scaled Planck constant and V is a given electrostatic potential. Problems related to equation (1.4) are of great interest in Physics and Engineering, since they describe models of solid state physics, *cf.*, *e.g.*, [5], Chapter 9, and [18], Chapter 5.

Finally, in the last section of the paper, we confirm the theoretical results of Sections 3 and 4 by investigating numerically the behaviour of the *a posteriori* error estimators.

2. Preliminaries

2.1. The Crank-Nicolson method

Let $0 = t^0 < t^1 < \cdots < t^N = T$ be a partition of $[0,T]$, $I_n := (t^{n-1}, t^n]$, $k_n := t^n - t^{n-1}$ and $k = \max_{1\le n\le N} k_n$. We discretize problem (1.1) only in time by the Crank-Nicolson method and we end up with approximations $U^n \in H_0^1(\Omega)$ to the values $u(t^n)$, $n = 0, 1, \ldots, N$, defined by

$$\bar{\partial} U^n - \mathrm{i}\alpha \Delta U^{n-\frac{1}{2}} + \mathrm{i} g\left(t^{n-\frac{1}{2}}\right) U^{n-\frac{1}{2}} = f\left(t^{n-\frac{1}{2}}\right), \quad n = 1, \ldots, N, \tag{2.1}$$

with $U^0 = u_0$. Here, we have used the notation

$$\bar{\partial} U^n := \frac{U^n - U^{n-1}}{k_n}, \quad U^{n-\frac{1}{2}} := \frac{U^n + U^{n-1}}{2} \quad \text{and} \quad t^{n-\frac{1}{2}} := \frac{t^n + t^{n-1}}{2} \cdot$$

The Crank-Nicolson method is of second order of accuracy. Thus, it is natural to define the continuous in time approximation $U(t)$ to $u(t)$, for $t \in [0,T]$, by linearly interpolating between the nodal values U^{n-1} and U^n. *I.e.*, $U : [0,T] \to H_0^1(\Omega)$ is defined by

$$U(t) := U^{n-\frac{1}{2}} + \left(t - t^{n-\frac{1}{2}}\right) \bar{\partial} U^n, \quad t \in I_n. \tag{2.2}$$

Then it is clear that, for $t \in [0,T]$, $u(t) - U(t) = O(k^2)$. However, as it was observed in [2], the use of this continuous approximation U in the *a posteriori* error analysis yields estimates of first instead of optimal second order of accuracy. Even in the case of $g \equiv 0$, the error $e := u - U$ satisfies the equation $e_t - \mathrm{i}\alpha\Delta e = -r$ with $r(t) := -\mathrm{i}\alpha(t - t^{n-\frac{1}{2}})\Delta\bar{\partial}U^n + \left[f(t^{n-\frac{1}{2}}) - f(t)\right]$, $t \in I_n$, *cf.* [2]. Then, r is an *a posteriori* quantity of first order. Thus, by applying energy techniques to the error equation $e_t - \mathrm{i}\alpha\Delta e = -r$, as in [8,20], we derive estimates of suboptimal order. That r is not of optimal order is due to the fact that it contains U_t and U_t $(U_t(t) = \bar{\partial}U^n$, $t \in I_n)$ is a first order approximation to u_t.

2.2. The Crank-Nicolson reconstruction

The Crank-Nicolson reconstruction $\hat{U} : [0,T] \to H^{-1}(\Omega)$ of U that we will use in the sequel, was the main tool in the analysis in [2]. This reconstruction is a piecewise quadratic polynomial defined by

$$\hat{U}(t) := U^{n-1} + \mathrm{i}\alpha\Delta \int_{t^{n-1}}^{t} U(s)\,\mathrm{d}s - \mathrm{i}\int_{t^{n-1}}^{t} G_U(t)\,\mathrm{d}t + \int_{t^{n-1}}^{t} F(t)\,\mathrm{d}t, \quad t \in I_n, \tag{2.3}$$

where $G_U : I_n \to L^2(\Omega)$ and $F : I_n \to L^2(\Omega)$ are the linear interpolants of gU and f, respectively, at the nodes t^{n-1} and $t^{n-\frac{1}{2}}$, *i.e.*,

$$G_U(t) := g\left(t^{n-\frac{1}{2}}\right) U^{n-\frac{1}{2}} + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left[g\left(t^{n-\frac{1}{2}}\right)U^{n-\frac{1}{2}} - g\left(t^{n-1}\right)U^{n-1}\right], \quad t \in I_n, \tag{2.4}$$

and

$$F(t) := f\left(t^{n-\frac{1}{2}}\right) + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left[f\left(t^{n-\frac{1}{2}}\right) - f\left(t^{n-1}\right)\right], \quad t \in I_n. \tag{2.5}$$

Note that to define the reconstruction $\hat{U}$ we use at each time interval I_n the Crank-Nicolson approximations U^{n-1} and U^n, $n = 1, \ldots, N$. This is the reason that this reconstruction is called "two point estimator". A three point Crank-Nicolson reconstruction is proposed in [16], *i.e.*, to define it at each I_n, we invoke the values U^{n-2}, U^{n-1} and U^n, $n = 2, \ldots, N$. The latter Crank-Nicolson reconstruction can be used alternatively to derive estimates of the same form as those we present in this paper.

From (2.3) we can easily see that $\hat{U}$ can be written as

$$\begin{aligned}\hat{U}(t) &= U^{n-1} + \mathrm{i}\frac{\alpha}{2}\left(t - t^{n-1}\right) \Delta \left(U(t) + U^{n-1}\right) \\ &+ \left(t - t^{n-1}\right)\left(f\left(t^{n-\frac{1}{2}}\right) - \mathrm{i}g\left(t^{n-\frac{1}{2}}\right)U^{n-\frac{1}{2}}\right) + \frac{1}{k_n}\left(t - t^{n-1}\right)\left(t^n - t\right) \\ &\times \left[\left(f\left(t^{n-\frac{1}{2}}\right) - f\left(t^{n-1}\right)\right) - \mathrm{i}\left(g\left(t^{n-\frac{1}{2}}\right)U^{n-\frac{1}{2}} - g\left(t^{n-1}\right)U^{n-1}\right)\right], \quad t \in I_n.\end{aligned} \tag{2.6}$$

Therefore, $\hat{U}(t^n) = U(t^n) = U^n$, $n = 0, 1, \ldots, N$. In particular, $\hat{U}$ is continuous. From (2.3) we also have that $\hat{U}$ satisfies

$$\hat{U}_t(t) - \mathrm{i}\alpha\Delta U(t) = -\mathrm{i}G_U(t) + F(t), \quad t \in I_n. \tag{2.7}$$

The *a posteriori* quantity $\hat{r}(t) := [\hat{U}_t - \mathrm{i}\alpha\Delta\hat{U} + \mathrm{i}g\hat{U} - f](t)$, $t \in I_n$, is the residual of $\hat{U}$. Using (2.7) we see that the residual can also be expressed as

$$\hat{r}(t) = -\mathrm{i}\alpha\Delta\left(\hat{U} - U\right)(t) + \mathrm{i}g(t)\left(\hat{U} - U\right)(t) + \mathrm{i}\left(gU - G_U\right)(t) + \left(F - f\right)(t), \ t \in I_n. \tag{2.8}$$

Furthermore, the difference $\hat{U}(t) - U(t)$, $t \in I_n$, can be written as in [2],

$$\begin{aligned}\hat{U}(t) - U(t) &= \frac{1}{2}\left(t - t^{n-1}\right)\left(t^n - t\right) \\ &\times \left[-\mathrm{i}\alpha\Delta\bar{\partial}U^n + \frac{2\mathrm{i}}{k_n}\left(g\left(t^{n-\frac{1}{2}}\right)U^{n-\frac{1}{2}} - g\left(t^{n-1}\right)U^{n-1}\right) - \frac{2}{k_n}\left(f\left(t^{n-\frac{1}{2}}\right) - f\left(t^{n-1}\right)\right)\right].\end{aligned} \tag{2.9}$$

Since $\{U^n\}_{n=0}^N$ are second order approximations to u at the nodes t^n, $n = 0, 1, \ldots, N$, we expect, in view of (2.9), that the difference $\hat{U} - U$ will be of second order of accuracy in time. Therefore, $\hat{r}(t) = O(k^2)$, $t \in [0, T]$. Thus, the use of the reconstruction $\hat{U}$ will lead to optimal bounds in the $L^\infty(L^2)$-norm, *cf.* Theorem 3.1 in the next section.

3. Estimate in the $L^\infty(L^2)$-norm

In this section we prove an optimal $L^\infty(L^2)$ *a posteriori* error estimate. In the analysis below, we would like the reconstruction $\hat{U}(t)$ to belong to $H_0^1(\Omega)$, for $t \in [0, T]$, and the residual $\hat{r}(t)$ to belong to $L^2(\Omega)$, for $t \in [0, T]$. From the definition of the residual (see also (2.8)), we see that a sufficient condition for $\hat{r}(t)$ to belong to $L^2(\Omega)$, for $t \in [0, T]$, is $\hat{U}(t) \in H^2(\Omega)$. Therefore, we would like to have $\hat{U}(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$. In general, the reconstruction we have defined in Section 2.2 does not belong to $H_0^1(\Omega) \cap H^2(\Omega)$, but to $H^{-1}(\Omega)$ instead. In order to ensure that $\hat{U}(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$, we may have to assume additional regularity and compatibility conditions on the data of the problem. In the following lemma we give *sufficient* conditions which ensure that $\hat{U}(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$.

Lemma 3.1. *For the data of problem* (1.2) *we further assume that*

$$\begin{cases} g(t) \in C^2(\bar{\Omega}), & \forall t \in [0, T] \ \textit{and} \\ \Delta u_0, f(t) \in H_0^1(\Omega) \cap H^2(\Omega), & \forall t \in [0, T]. \end{cases}$$

Then $\hat{U}(t) \in H_0^1(\Omega) \cap H^2(\Omega)$.

Proof. The regularity and compatibility assumptions on the data of problem (1.2) ensure that $U^n \in H_0^1(\Omega) \cap H^2(\Omega)$, $n = 0, 1, \dots, N$, in light of the method (2.1). Therefore, $g(t^{n-\frac{1}{2}})U^{n-\frac{1}{2}} \in H_0^1(\Omega) \cap H^2(\Omega)$ because $g(t) \in C^2(\bar{\Omega})$, for $t \in [0, T]$. Using once more (2.1) and the fact that $f(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$, we immediately obtain that $\Delta U^{n-\frac{1}{2}} \in H_0^1(\Omega) \cap H^2(\Omega)$, $n = 1, \dots, N$. Since $\Delta U^0 = \Delta u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$, an inductive argument ensures that $\Delta U^n \in H_0^1(\Omega) \cap H^2(\Omega)$, $n = 0, 1, \dots, N$. This yields $\Delta U(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$. On the other hand it is easily seen that $G_U(t), F(t) \in H_0^1(\Omega) \cap H^2(\Omega)$, for $t \in [0, T]$, and the proof is complete, in view of (2.3). □

Remark 3.1. Condition $\Delta u_0 \in H_0^1(\Omega)$ is actually needed in order to ensure that U^n, $n = 1, \dots, N$, are indeed second order approximations to u at the nodes t^n, $n = 1, \dots, N$ (see for example [19], Chap. 7).

Remark 3.2. A more detailed analysis about when the reconstruction $\hat{U}$ belongs to the correct space can be found in [3]. However, we would like to point out that in cases of fully discrete schemes, the reconstruction and the residual belong to the spaces $H_0^1(\Omega)$ and $L^2(\Omega)$, respectively, without further assumptions on the data of the problem (see for example [11], or [14], Second Part). Therefore, from now on we will assume that $\hat{U} : [0, T] \to H_0^1(\Omega)$ and $\hat{r} : [0, T] \to L^2(\Omega)$.

We are now ready to derive the estimate in the $L^\infty(L^2)$-norm. Let the error $\hat{e} : [0, T] \to H_0^1(\Omega)$ be defined by $\hat{e} := u - \hat{U}$. By the residual's definition and problem (1.1) we conclude, for $t \in I_n$, $n = 1, \dots, N$, that the error satisfies, in weak form, the problem

$$\begin{cases} (\hat{e}_t(t), \upsilon) + \mathrm{i}\alpha(\nabla\hat{e}(t), \nabla\upsilon) + \mathrm{i}\big(g(t)\hat{e}(t), \upsilon\big) = -\big(\hat{r}(t), \upsilon\big), & \forall \upsilon \in H_0^1(\Omega), \\ \hat{e}(\cdot, 0) = 0, & \text{in } \bar{\Omega}. \end{cases} \tag{3.1}$$

Setting in (3.1) $\upsilon = \hat{e}$, then taking real parts and using the Cauchy-Schwarz inequality we arrive at

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\hat{e}(t)\|_{L^2(\Omega)}^2 \le \|\hat{r}(t)\|_{L^2(\Omega)}\|\hat{e}(t)\|_{L^2(\Omega)},$$

or,

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\hat{e}(t)\|_{L^2(\Omega)} \le \|\hat{r}(t)\|_{L^2(\Omega)}.$$

Integrating the above relation from 0 to t^n, $n = 1, \dots, N$, we immediately obtain the following:

Theorem 3.1 (*a posteriori* error estimate in the $L^\infty(L^2)$-norm)**.** *Let u be the weak solution of problem* (1.1)*, $\hat{U}$ the Crank-Nicolson reconstruction* (2.3) *and $\hat{e} = u - \hat{U}$. Then the following optimal order* a posteriori *error estimate holds for $n = 1, \dots, N$,*

$$\max_{0 \le t \le t^n} \|\hat{e}(t)\|_{L^2(\Omega)} \le \int_0^{t^n} \|\hat{r}(t)\|_{L^2(\Omega)}\,\mathrm{d}t, \tag{3.2}$$

where the a posteriori *quantity $\hat{r}$ is given by* (2.8).

In the next section we will see that the error equation (3.1) is not sufficient to control the error in the $L^\infty(H^1)$-norm in an optimal way.

4. *A posteriori* error estimates in the $L^\infty(H^1)$-norm

To obtain estimates in the $L^\infty(H^1)$-norm we need further regularity for the solution u of problem (1.2). In particular, in this section, in addition to the conditions (1.3) we assume that

$$\begin{cases} g_{tt} \in L^2\big([0, T]; L^2(\Omega)\big), \\ f \in L^2\big([0, T]; H^1(\Omega)\big),\ f_t \in L^2\big([0, T]; L^2(\Omega)\big),\ f_{tt} \in L^2\big([0, T]; H^{-1}(\Omega)\big), \\ \mathrm{i}\alpha\Delta u_0 + f(0) \in H_0^1(\Omega). \end{cases} \tag{4.1}$$

Then it can be proven that $u \in C\big([0,T]; H_0^1(\Omega)\cap H^2(\Omega)\big)$, $u_t \in C\big([0,T]; H_0^1(\Omega)\big)$ and $u_{tt} \in C\big([0,T]; H^{-1}(\Omega)\big)$. The proof of this statement follows similar arguments to those in the proof of Theorems 5 and 6, pp. 389–393, in [9], it is beyond the scope of the paper and thus it is omitted.

The starting point to derive estimates in the $L^\infty(H^1)$-norm is equation (3.1). Indeed, setting $\upsilon = \hat{e}_t$ in (3.1) and then taking imaginary parts, we get

$$\frac{\alpha}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla\hat{e}(t)\|^2_{L^2(\Omega)} \le \Big(\sup_{x\in\Omega}|g(x,t)|\,\|\hat{e}(t)\|_{L^2(\Omega)} + \|\hat{r}(t)\|_{L^2(\Omega)}\Big)\|\hat{e}_t(t)\|_{L^2(\Omega)}, \quad t\in I_n. \tag{4.2}$$

From (4.2), it is clear that to estimate $\|\nabla\hat{e}(t)\|_{L^2(\Omega)}$, we must control the quantity $\|\hat{e}_t(t)\|_{L^2(\Omega)}$.

4.1. **First order estimates**

To control $\|\hat{e}_t(t)\|_{L^2(\Omega)}$, we differentiate (2.6) to obtain

$$\begin{aligned}\hat{U}_t(t) &= \mathrm{i}\alpha\Delta U^{n-1} + \mathrm{i}\alpha\left(t-t^{n-1}\right)\Delta\bar{\partial}U^n\\ &\quad -\mathrm{i}\left\{g\left(t^{n-\frac12}\right)U^{n-\frac12} + \frac{2}{k_n}\left(t-t^{n-\frac12}\right)\left(g\left(t^{n-\frac12}\right)U^{n-\frac12} - g\left(t^{n-1}\right)U^{n-1}\right)\right\}\\ &\quad +\left\{f\left(t^{n-\frac12}\right) - \frac{2}{k_n}\left(t-t^{n-\frac12}\right)\left(f\left(t^{n-\frac12}\right)-f\left(t^{n-1}\right)\right)\right\}, \quad t\in I_n.\end{aligned} \tag{4.3}$$

At this point, a careful analysis is needed, since $\hat{U}_t$ is discontinuous at the nodes t^n, $n=1,\dots,N-1$. Indeed, it is easily seen that

$$\hat{U}_t(t^{n-}) = \mathrm{i}\alpha\Delta U^n - \mathrm{i}\left(2g\left(t^{n-\frac12}\right)U^{n-\frac12} + g\left(t^{n-1}\right)U^{n-1}\right) + \left(2f\left(t^{n-\frac12}\right) - f\left(t^{n-1}\right)\right)$$

and

$$\hat{U}_t(t^{n+}) = \mathrm{i}\alpha\Delta U^n - \mathrm{i}g(t^n)U^n + f(t^n).$$

Therefore, in general, $\hat{U}_t(t^{n-}) \ne \hat{U}_t(t^{n+})$. However, we can conclude that

$$\hat{U}_t(t^{n+}) - \hat{U}_t(t^{n-}) = O\left(k^2\right), \quad n=1,\dots,N-1. \tag{4.4}$$

It is to be emphasized that (4.4) is crucial to deduce the order of the upper bound in the estimate (4.9) below. By differentiation of (3.1), we get, for $t\in I_n$, $n=1,\dots,N$,

$$\big(\hat{e}_{tt}(t),\upsilon\big) + \mathrm{i}\alpha\big(\nabla\hat{e}_t(t),\nabla\upsilon\big) + \mathrm{i}\big(g(t)\hat{e}_t(t),\upsilon\big) = -\mathrm{i}\big(g_t(t)\hat{e}(t),\upsilon\big) - \big(\hat{r}_t(t),\upsilon\big), \quad \forall\upsilon\in H_0^1(\Omega). \tag{4.5}$$

Thus, by taking in (4.5) $\upsilon = \hat{e}_t$, then real parts and integrating from t^{n-1} to t, we obtain

$$\begin{aligned}\|\hat{e}_t(t)\|_{L^2(\Omega)} \le \left\|\hat{e}_t\left(t^{(n-1)+}\right)\right\|_{L^2(\Omega)} &+ \max_{t^{n-1}\le t\le t^n}\|\hat{e}(t)\|_{L^2(\Omega)}\int_{t^{n-1}}^{t^n}\sup_{x\in\Omega}|g_t(x,t)|\,\mathrm{d}t\\ &+\int_{t^{n-1}}^{t^n}\|\hat{r}_t(t)\|_{L^2(\Omega)}\,\mathrm{d}t, \quad t\in I_n.\end{aligned} \tag{4.6}$$

Notice now that the following inequality holds for $n=1,\dots,N$,

$$\left\|\hat{e}_t\left(t^{(n-1)+}\right)\right\|_{L^2(\Omega)} \le \left\|\hat{e}_t\left(t^{(n-1)-}\right)\right\|_{L^2(\Omega)} + \left\|\hat{U}_t\left(t^{(n-1)+}\right) - \hat{U}_t\left(t^{(n-1)-}\right)\right\|_{L^2(\Omega)}, \tag{4.7}$$

because u_t is a time-continuous function, *cf.* Introduction. In view of (4.7), (4.6) is rewritten as

$$\|\hat{e}_t(t)\|_{L^2(\Omega)} \le \left\|\hat{e}_t\left(t^{(n-1)-}\right)\right\|_{L^2(\Omega)} + \left\|\hat{U}_t\left(t^{(n-1)+}\right) - \hat{U}_t\left(t^{(n-1)-}\right)\right\|_{L^2(\Omega)} + \max_{t^{n-1}\le t\le t^n}\|\hat{e}(t)\|_{L^2(\Omega)}\int_{t^{n-1}}^{t^n}\sup_{x\in\Omega}|g_t(x,t)|\,\mathrm{d}t + \int_{t^{n-1}}^{t^n}\|\hat{r}_t(t)\|_{L^2(\Omega)}\,\mathrm{d}t,\ \ t\in I_n,$$

and therefore, using induction we conclude the estimate (we implicitly set $\sum_{m=1}^{0} := 0$)

$$\begin{aligned}\|\hat{e}_t(t)\|_{L^2(\Omega)} \le \|\hat{e}_t(0)\|_{L^2(\Omega)} + \sum_{m=1}^{n-1}\left\|\hat{U}_t\left(t^{m+}\right) - \hat{U}_t\left(t^{m-}\right)\right\|_{L^2(\Omega)} \\ + \max_{0\le t\le t^n}\|\hat{e}(t)\|_{L^2(\Omega)}\int_0^{t^n}\sup_{x\in\Omega}|g_t(x,t)|\,\mathrm{d}t + \int_0^{t^n}\|\hat{r}_t(t)\|_{L^2(\Omega)}\,\mathrm{d}t, \quad t\in I_n.\end{aligned} \tag{4.8}$$

Since $\hat{e}(0)=0$ and $\hat{r}(0)=0$ we have, in view of (3.1), that $\hat{e}_t(0)=0$ as well. Hence (4.8) is now written, in light of (3.2), as

$$\begin{aligned}\sup_{0\le t\le t^n}\|\hat{e}_t(t)\|_{L^2(\Omega)} \le \sum_{m=1}^{n-1}\|\hat{U}_t(t^{m+}) - \hat{U}_t(t^{m-})\|_{L^2(\Omega)} \\ + \int_0^{t^n}\sup_{x\in\Omega}|g_t(x,t)|\,\mathrm{d}t\int_0^{t^n}\|\hat{r}(t)\|_{L^2(\Omega)}\,\mathrm{d}t + \int_0^{t^n}\|\hat{r}_t(t)\|_{L^2(\Omega)}\,\mathrm{d}t.\end{aligned} \tag{4.9}$$

Remark 4.1. Relation (4.9) gives an *a posteriori* estimate for $\hat{e}_t$ in the $L^\infty(L^2)$-norm of first order. This is because both terms $\sum_{m=1}^{n-1}\|\hat{U}_t(t^{m+}) - \hat{U}_t(t^{m-})\|_{L^2(\Omega)}$ and $\int_0^{t^n}\|\hat{r}_t(t)\|_{L^2(\Omega)}\,dt$ are in general of first instead of second order of accuracy. This immediately follows from (4.4) for the first term while for the second, this can be verified by differentiation in time of (2.8). Even in the simplest case when $g\equiv 0$ and $f\equiv 0$ we have $\hat{r}_t(t)=O(k)$. Indeed, in this case, it is easily seen that

$$\hat{r}_t(t) = \mathrm{i}\frac{\alpha}{2}\left(2t - t^{n-1} - t^n\right)\Delta\bar{\partial}U^n, \quad t\in I_n,$$

and therefore, in general, $\hat{r}_t(t)=O(k)$.

Invoking in (4.2) the estimates (3.2), (4.9) and integrating from 0 to t^n we conclude to:

Theorem 4.1 (suboptimal *a posteriori* error estimate in $L^\infty(H^1)$- norm)**.** *With the notation of Theorem 3.1 the following* a posteriori *error estimate is valid, for $n=1,\ldots,N$,*

$$\begin{aligned}\max_{0\le t\le t^n}\|\nabla\hat{e}(t)\|^2_{L^2(\Omega)} \le \frac{2}{\alpha}\left(1+\int_0^{t^n}\sup_{x\in\Omega}|g(x,t)|\,\mathrm{d}t\right) \\ \times\int_0^{t^n}\|\hat{r}(t)\|_{L^2(\Omega)}\,\mathrm{d}t\sup_{0\le t\le t^n}\|\hat{e}_t(t)\|_{L^2(\Omega)},\end{aligned} \tag{4.10}$$

where the quantity $\sup_{0\le t\le t^n}\|\hat{e}_t(t)\|_{L^2(\Omega)}$ is estimated a posteriori via (4.9).

Theorem 4.1 yields an *a posteriori* error estimate in the $L^\infty(H^1)$-norm of order $\frac{3}{2}$ in time, instead of two, which is the optimal order of accuracy. To recover the optimal order we have to proceed in a different way and to introduce new ideas. This will be the topic of the next subsection.

4.2. **Recovery of optimality**

The main idea of the proof of optimal order *a posteriori* estimates in the $L^\infty(H^1)$-norm is based on considering the auxiliary initial- and boundary-value problem:

$$\begin{cases} w_t - \mathrm{i}\alpha\Delta w + \mathrm{i}g(x,t)w = f_t(x,t) - \mathrm{i}g_t(x,t)\hat{U} & \text{in } \bar{\Omega}\times[0,T], \\ w = 0 & \text{on } \partial\Omega\times[0,T], \\ w(\cdot,0) = \mathrm{i}\alpha\Delta u_0 - \mathrm{i}g(\cdot,0)u_0 + f(\cdot,0) & \text{in } \bar{\Omega}. \end{cases} \tag{4.11}$$

Since $\hat{U}$ is a piecewise quadratic polynomial with $\hat{U}(t), \hat{U}_t(t) \in L^2(\Omega)$, for almost every $t \in [0,T]$, it can be proven (*cf.* [7], pp. 620–630) that, under conditions (1.3) and (4.1), problem (4.11) has a unique solution $w \in C\big([0,T]; H_0^1(\Omega)\big)$ with $w_t \in C\big([0,T]; H^{-1}(\Omega)\big)$.

Note that since $\hat{U}$ is a second order approximation to u, and u_t satisfies the following problem:

$$\begin{cases} (u_t)_t - \mathrm{i}\alpha\Delta u_t + \mathrm{i}g(x,t)u_t = f_t(x,t) - \mathrm{i}g_t(x,t)u & \text{in } \bar{\Omega}\times[0,T], \\ u_t = 0 & \text{on } \partial\Omega\times[0,T], \\ u_t(\cdot,0) = \mathrm{i}\alpha\Delta u_0 - \mathrm{i}g(\cdot,0)u_0 + f(\cdot,0) & \text{in } \bar{\Omega}, \end{cases} \tag{4.12}$$

we expect that w will be a second order approximation to u_t, see Lemma 4.1 below.

We discretize problem (4.11) by the Crank-Nicolson method, *i.e.*, we derive approximations W^n, $n = 0,1,\ldots,N$, defined by

$$\begin{cases} \bar{\partial}W^n - \mathrm{i}\alpha\Delta W^{n-\frac12} + \mathrm{i}g\left(t^{n-\frac12}\right)W^{n-\frac12} = f_t\left(t^{n-\frac12}\right) - \mathrm{i}g_t\left(t^{n-\frac12}\right)\hat{U}\left(t^{n-\frac12}\right), \\ W^0 = \mathrm{i}\alpha\Delta u_0 - \mathrm{i}g(0)u_0 + f(0) \quad \text{in } \bar{\Omega}. \end{cases} \tag{4.13}$$

Let $W : [0,T] \to H_0^1(\Omega)$ be the Crank-Nicolson approximation to w, *i.e.*, the linear interpolate between the nodal values W^{n-1} and W^n,

$$W(t) := W^{n-\frac12} + \left(t - t^{n-\frac12}\right)\bar{\partial}W^n, \quad t \in I_n.$$

Also let $\hat{W} : [0,T] \to H_0^1(\Omega)$ be the Crank-Nicolson reconstruction of W,

$$\begin{aligned} \hat{W}(t) = {} & W^{n-1} + \mathrm{i}\alpha\left(t - t^{n-1}\right)\Delta W^{n-1} + \mathrm{i}\frac{\alpha}{2}\left(t - t^{n-1}\right)^2\Delta\bar{\partial}W^n \\ & - \mathrm{i}\left(t - t^{n-1}\right)g\left(t^{n-\frac12}\right)W^{n-\frac12} \\ & - \frac{\mathrm{i}}{k_n}\left(t - t^{n-1}\right)\left(t^n - t\right)\left(g\left(t^{n-\frac12}\right)W^{n-\frac12} - g\left(t^{n-1}\right)W^{n-1}\right) \\ & - \mathrm{i}\left(t - t^{n-1}\right)g_t\left(t^{n-\frac12}\right)\hat{U}\left(t^{n-\frac12}\right) \\ & - \frac{\mathrm{i}}{k_n}\left(t - t^{n-1}\right)\left(t^n - t\right)\left(g_t\left(t^{n-\frac12}\right)\hat{U}\left(t^{n-\frac12}\right) - g_t\left(t^{n-1}\right)U^{n-1}\right) \\ & + \left(t - t^{n-1}\right)f_t\left(t^{n-\frac12}\right) \\ & + \frac{1}{k_n}\left(t - t^{n-1}\right)\left(t^n - t\right)\left(f_t\left(t^{n-\frac12}\right) - f_t\left(t^{n-1}\right)\right), \quad t \in I_n. \end{aligned} \tag{4.14}$$

Note that the new reconstruction $\hat{W}$ we have just defined depends on the reconstruction $\hat{U}$.

As in the definition of the residual $\hat{r}$ for the reconstruction $\hat{U}$, we define the residual $\hat{R} : [0,T] \to L^2(\Omega)$ for $\hat{W}$ as

$$\hat{R}(t) := (\hat{W}_t - \mathrm{i}\alpha\Delta\hat{W} + \mathrm{i}g\hat{W} - f_t + \mathrm{i}g_t\hat{U})(t), \quad t \in I_n,\, n = 1,\dots,N. \tag{4.15}$$

Remark 4.2. Here we assume again that $\hat{W}(t) \in H_0^1(\Omega)$ and $\hat{R}(t) \in L^2(\Omega)$, for $t \in [0,T]$. As in Section 3, to ensure this we might need to assume additional regularity and compatibility conditions on the data of problem (4.11), in the spirit of Lemma 3.1. However, we point out once more that in the cases of fully discrete schemes, no further conditions are required to ensure that $\hat{W}(t) \in H_0^1(\Omega)$ and $\hat{R}(t) \in L^2(\Omega)$, for $t \in [0,T]$.

Since problem (4.11) is of the same form as problem (1.1) with the function f replaced by the function $f_t - \mathrm{i}g_t\hat{U}$ and the initial value u_0 replaced by $\mathrm{i}\alpha\Delta u_0 - \mathrm{i}g(0)u_0 + f(0)$, we have, according to (2.3)–(2.5), that the residual $\hat{R}$ is written for $t \in I_n$, $n = 1,\dots,N$, as

$$\begin{aligned}\hat{R}(t) = &-\mathrm{i}\alpha\Delta\left(\hat{W} - W\right)(t) + \mathrm{i}g(t)\left(\hat{W} - W\right)(t) + \mathrm{i}\big(g(t)W(t) - G_W(t)\big)\\ &+\left(\tilde{F}(t) - f_t(t)\right) + \mathrm{i}\left(g_t(t)\hat{U}(t) - \tilde{G}_{\hat{U}}(t)\right),\end{aligned} \tag{4.16}$$

with

$$G_W(t) := g\left(t^{n-\frac{1}{2}}\right)W^{n-\frac{1}{2}} + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left[g\left(t^{n-\frac{1}{2}}\right)W^{n-\frac{1}{2}} - g\left(t^{n-1}\right)W^{n-1}\right], \tag{4.17}$$

$$\tilde{F}(t) := f_t\left(t^{n-\frac{1}{2}}\right) + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left[f_t\left(t^{n-\frac{1}{2}}\right) - f_t\left(t^{n-1}\right)\right] \tag{4.18}$$

and

$$\tilde{G}_{\hat{U}}(t) := \mathrm{i}g_t\left(t^{n-\frac{1}{2}}\right)\hat{U}\left(t^{n-\frac{1}{2}}\right) + \frac{2\mathrm{i}}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left[g_t\left(t^{n-\frac{1}{2}}\right)\hat{U}\left(t^{n-\frac{1}{2}}\right) - g_t\left(t^{n-1}\right)U^{n-1}\right], \tag{4.19}$$

Also recall that for $t \in I_n$, $n = 1,\dots,N$,

$$\begin{aligned}\hat{W}(t) - W(t) = \frac{1}{2}\left(t - t^{n-1}\right)\left(t^n - t\right)\Bigg[&-\mathrm{i}\alpha\Delta\bar{\partial}W^n + \frac{2\mathrm{i}}{k_n}\left(g\left(t^{n-\frac{1}{2}}\right)W^{n-\frac{1}{2}} - g\left(t^{n-1}\right)W^{n-1}\right)\\ &-\frac{2}{k_n}\left(f_t\left(t^{n-\frac{1}{2}}\right) - f_t\left(t^{n-1}\right)\right) + \frac{2\mathrm{i}}{k_n}\left(g_t\left(t^{n-\frac{1}{2}}\right)\hat{U}\left(t^{n-\frac{1}{2}}\right) - g_t\left(t^{n-1}\right)U^{n-1}\right)\Bigg].\end{aligned} \tag{4.20}$$

Since the first and the second time-derivative of $\hat{U}$ are discontinuous functions at the nodes t^n, $n = 1,\dots, N-1$, it is not obvious that the Crank-Nicolson approximations W^n are second order approximations to the values $w(t^n)$, $n = 1,\dots,N$, even if the data of the problem are compatible and smooth enough. So, for completeness, we will prove that the Crank-Nicolson approximations W^n are indeed second order approximations to the values $w(t^n)$, $n = 1,\dots,N$.

Lemma 4.1. *Let u and w be the weak solutions of problems* (1.1) *and* (4.11)*, respectively. Then, for $n = 1,\dots,N$,*

$$\max_{0\le t\le t^n}\|(u_t - w)(t)\|_{L^2(\Omega)} \le \int_0^{t^n}\sup_{x\in\Omega}|g_t(x,t)|\,\mathrm{d}t\int_0^{t^n}\|\hat{r}(t)\|_{L^2(\Omega)}\,\mathrm{d}t, \tag{4.21}$$

where $\hat{r}$ is the residual given by (2.8).

Proof. It is easily seen that the difference $u_t - w$ satisfies the problem

$$\begin{cases}\big((u_t - w)_t(t), \upsilon\big) + \mathrm{i}\alpha\big(\nabla(u_t - w)(t), \nabla\upsilon\big) + \mathrm{i}\big(g(t)(u_t - w)(t), \upsilon\big)\\ \qquad\qquad = -\mathrm{i}\big(g_t(t)\hat{e}(t), \upsilon\big), \quad \forall\upsilon \in H_0^1(\Omega),\, t \in I_n,\\ (u_t - w)(0) = 0, \text{ in } \bar{\Omega}.\end{cases} \tag{4.22}$$

Choosing in (4.22) $v = u_t - w$, then taking real parts, and integrating from 0 to t^n, we obtain

$$\max_{0\le t\le t^n} \|(u_t - w)(t)\|_{L^2(\Omega)} \le \int_0^{t^n} \sup_{x\in\Omega} |g_t(x,t)|\,\mathrm{d}t \max_{0\le t\le t^n} \|\hat{e}(t)\|_{L^2(\Omega)}. \tag{4.23}$$

Estimate (4.23) yields estimate (4.21) in view of (3.2). □

In the proposition below, we prove that the W^n are second order approximations to w at the nodes t^n, $n = 1,\dots,N$. The idea of the proof is based on splitting the error $W^n - w(t^n)$ as

$$W^n - w(t^n) = \left(W^n - \tilde{W}^n\right) + \left(\tilde{W}^n - u_t(t^n)\right) + (u_t - w)(t^n) \tag{4.24}$$

where the $\{\tilde{W}^n\}_{n=0}^N$ denote the Crank-Nicolson approximations which correspond to problem (4.12),

$$\begin{cases} \bar{\partial}\tilde{W}^n - \mathrm{i}\alpha\Delta\tilde{W}^{n-\frac12} + \mathrm{i}g(t^{n-\frac12})\tilde{W}^{n-\frac12} \\ \qquad\qquad = f_t(t^{n-\frac12}) - \mathrm{i}g_t(t^{n-\frac12})u(t^{n-\frac12}), \quad n = 1,\dots,N, \\ \tilde{W}^0 = W^0 \quad \text{in } \bar{\Omega}. \end{cases} \tag{4.25}$$

Proposition 4.1. *Let w be the (weak) solution of problem (4.11) and W^n be the Crank-Nicolson approximations of w at the nodes t^n, $n = 0,1,\dots,N$, defined by the numerical scheme (4.13). Then, if*

$$\max_{0\le n\le N} \left\|u_t(t^n) - \tilde{W}^n\right\|_{L^2(\Omega)} = O(k^2), \tag{4.26}$$

we have that

$$\max_{0\le n\le N} \|W^n - w(t^n)\|_{L^2(\Omega)} = O(k^2).$$

Proof. We set $Z^n := W^n - \tilde{W}^n$, $n = 0,1,\dots,N$. Using the schemes (4.13) and (4.25) we have that the Z^n, $n = 0,1,\dots,N$, satisfy the following numerical scheme

$$\begin{cases} \bar{\partial}Z^n - \mathrm{i}\alpha\Delta Z^{n-\frac12} + \mathrm{i}g\left(t^{n-\frac12}\right)Z^{n-\frac12} = \mathrm{i}g_t\left(t^{n-\frac12}\right)\hat{e}\left(t^{n-\frac12}\right), \quad n = 1,\dots,N, \\ Z^0 = 0 \quad \text{in } \bar{\Omega}. \end{cases} \tag{4.27}$$

Applying standard stability arguments in (4.27) we can easily conclude that

$$\max_{0\le n\le N} \|Z^n\|_{L^2(\Omega)} \le C(\|Z^0\|_{L^2(\Omega)} + \max_{0\le t\le T} \|\hat{e}(t)\|_{L^2(\Omega)}), \tag{4.28}$$

where the constant C depends only on the final time T and g_t. Accordingly,

$$\max_{0\le n\le N} \left\|W^n - \tilde{W}^n\right\|_{L^2(\Omega)} = O(k^2)$$

and the proof is complete in light of (4.21), (4.24) and (4.26). □

Corollary 4.1. *The residual $\hat{R} : [0,T] \to L^2(\Omega)$ defined in (4.15) and corresponding to the reconstruction $\hat{W}$ is of second order of accuracy in time.*

We recall that our goal is to prove *a posteriori* error estimates of optimal (second) order of accuracy for the quantity $\sup_{0\le t\le t^n} \|\hat{e}_t(t)\|_{L^2(\Omega)}$, $n = 1,\dots,N$. To achieve this, we split the error $\hat{e}_t$ as

$$\hat{e}_t = (u_t - w) + \left(w - \hat{W}\right) + \left(\hat{W} - \hat{U}_t\right).$$

The quantity $u_t - w$ is estimated *a posteriori* in the $L^\infty(L^2)$-norm *via* the optimal order estimate (4.21), while $\hat{W} - \hat{U}_t$ is already an *a posteriori* quantity. For the quantity $w - \hat{W}$ we use the following:

Lemma 4.2. *Let w be the (weak) solution of problem (4.11) and $\hat{W}$ the corresponding Crank-Nicolson reconstruction. Then, for $n = 1, \dots, N$, the following* a posteriori *estimate is valid for the error $w - \hat{W}$ in the $L^\infty(L^2)$-norm*

$$\max_{0\le t\le t^n} \left\| \left(w - \hat{W}\right)(t) \right\|_{L^2(\Omega)} \le \int_0^{t^n} \left\| \hat{R}(t) \right\|_{L^2(\Omega)} \mathrm{d}t, \tag{4.29}$$

where $\hat{R} : [0,T] \to L^2(\Omega)$ is the residual given by (4.15).

Using Lemmata 4.1 and 4.2 we can prove the following:

Theorem 4.2 (*a posteriori* estimate of optimal order for $\sup_{0\le t\le T} \|\hat{e}_t(t)\|_{L^2(\Omega)}$)**.** *With the notation of Theorem 3.1, the following* a posteriori *error estimate holds, for $n = 1, \dots, N$,*

$$\begin{aligned} \sup_{0\le t\le t^n} \|\hat{e}_t(t)\|_{L^2(\Omega)} \le & \int_0^{t^n} \sup_{x\in\Omega} |g_t(x,t)| \,\mathrm{d}t \int_0^{t^n} \|\hat{r}(t)\|_{L^2(\Omega)} \,\mathrm{d}t \\ & + \int_0^{t^n} \|\hat{R}(t)\|_{L^2(\Omega)} \,\mathrm{d}t + \sup_{0\le t\le t^n} \left\|\hat{W}(t) - \hat{U}_t(t)\right\|_{L^2(\Omega)}, \end{aligned} \tag{4.30}$$

where the residuals $\hat{r}$ and $\hat{R}$ are given by (2.8) and (4.16), respectively, and $\hat{W}$ is the Crank-Nicolson reconstruction corresponding to problem (4.11).

We are now ready to formulate the basic theorem of this section.

Theorem 4.3 (*a posteriori* error estimate of optimal order in the $L^\infty(H^1)$-norm)**.** *With the notation of the previous theorem, the following a posteriori error estimate holds, for $n = 1, \dots, N$,*

$$\begin{aligned} \max_{0\le t\le t^n} \|\nabla \hat{e}(t)\|^2_{L^2(\Omega)} \le & \frac{2}{\alpha} \left(1 + \int_0^{t^n} \sup_{x\in\Omega} |g(x,t)| \,\mathrm{d}t\right) \\ & \times \int_0^{t^n} \|\hat{r}(t)\|_{L^2(\Omega)} \,\mathrm{d}t \sup_{0\le t\le t^n} \|\hat{e}_t(t)\|_{L^2(\Omega)}, \end{aligned} \tag{4.31}$$

where the quantity $\sup_{0\le t\le t^n} \|\hat{e}_t(t)\|$ is estimated by the optimal order *estimate (4.30).*

In Theorems 4.2 and 4.3 we claim that estimates (4.30) and (4.31) are of optimal second order. This is true if $\hat{W}$ is a second order approximation in time to $\hat{U}_t$. We prove this in Lemma 4.3 below, using *a priori* error analysis. However, we emphasize that estimates (4.30) and (4.31) are valid *independently* of Lemma 4.3. Since $\hat{W} - \hat{U}_t$ is an *a posteriori* quantity, the order of $\sup_{0\le t\le T} \|(\hat{W} - \hat{U}_t)(t)\|_{L^2(\Omega)}$ can always be checked numerically.

Lemma 4.3. *Let $\hat{U}$ be the Crank-Nicolson reconstruction given in (2.6) and corresponding to problem (1.1) and let $\hat{W}$ be the Crank-Nicolson reconstruction given in (4.14) and corresponding to problem (4.11). Then*

$$\sup_{0\le t\le T} \left\| \left(\hat{W} - \hat{U}_t\right)(t) \right\|_{L^2(\Omega)} = O\left(k^2\right).$$

Proof. According to (4.3) and (4.14) it suffices to prove that for $t \in I_n$, $n = 1, \ldots, N$,

$$\begin{aligned}
&\mathrm{i}\alpha \Delta U^{n-1} + \mathrm{i}\alpha \left(t - t^{n-1}\right) \Delta \bar{\partial} U^n \\
&- \mathrm{i}\left[g\left(t^{n-\frac{1}{2}}\right) U^{n-\frac{1}{2}} + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left(g\left(t^{n-\frac{1}{2}}\right) U^{n-\frac{1}{2}} - g\left(t^{n-1}\right) U^{n-1}\right)\right] \\
&+ \left[f\left(t^{n-\frac{1}{2}}\right) + \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left(f\left(t^{n-\frac{1}{2}}\right) - f\left(t^{n-1}\right)\right)\right] - (t - t^{n-1}) f_t(t^{n-\frac{1}{2}}) \\
&- W^{n-1} - \mathrm{i}\alpha \left(t - t^{n-1}\right) \Delta W^{n-1} + \mathrm{i}\left(t - t^{n-1}\right) g\left(t^{n-\frac{1}{2}}\right) W^{n-\frac{1}{2}} \\
&+ \mathrm{i}\left(t - t^{n-1}\right) g_t\left(t^{n-\frac{1}{2}}\right) \hat{U}\left(t^{n-\frac{1}{2}}\right) = O\left(k^2\right).
\end{aligned} \tag{4.32}$$

Using (4.21) and the fact that the Crank-Nicolson approximations U^n and W^n are of second order approximations to the values $u(t^n)$ and $w(t^n)$, respectively, we can easily derive for $n = 1, \ldots, N$,

$$\mathrm{i}\alpha \left(t - t^{n-1}\right) \Delta \left(\bar{\partial} U^n - W^{n-1}\right) = O\left(k^2\right) \tag{4.33}$$

and

$$\mathrm{i}\alpha \Delta U^{n-1} - W^{n-1} = \mathrm{i}g\left(t^{n-1}\right) U^{n-1} - f\left(t^{n-1}\right) + O\left(k^2\right), \quad n = 1, \ldots, N. \tag{4.34}$$

Furthermore, for $\mathcal{F}$ smooth it holds

$$\begin{aligned}
&\mathcal{F}(t^{n-1}) + \left(t - t^{n-1}\right) \mathcal{F}_t\left(t^{n-\frac{1}{2}}\right) - \mathcal{F}\left(t^{n-\frac{1}{2}}\right) \\
&\qquad - \frac{2}{k_n}\left(t - t^{n-\frac{1}{2}}\right)\left(\mathcal{F}\left(t^{n-\frac{1}{2}}\right) - \mathcal{F}\left(t^{n-1}\right)\right) = O\left(k^2\right).
\end{aligned} \tag{4.35}$$

Combining estimates (4.33)–(4.35) for $\mathcal{F} = f$ and $\mathcal{F} = gu$ we immediately conclude (4.32) and the proof is complete. □

Remark 4.3. Note that the second order terms of (4.14) have been absorbed in the right-hand side of (4.32).

Remark 4.4. The difference between the estimates (4.9) and (4.30) is that the suboptimal order term

$$\sum_{m=1}^{n-1} \left\| \hat{U}_t(t^{m+}) - \hat{U}_t(t^{m-}) \right\|_{L^2(\Omega)} + \int_0^{t^n} \|\hat{r}_t(t)\|_{L^2(\Omega)} \,\mathrm{d}t$$

in (4.9) is replaced by the optimal order term

$$\sup_{0 \le t \le t^n} \left\| W(t) - \hat{U}_t(t) \right\|_{L^2(\Omega)} + \int_0^{t^n} \left\| \hat{R}(t) \right\|_{L^2(\Omega)} \mathrm{d}t.$$

Notice also that even though in the estimate (4.30) we have a recovery of optimality, we also need to compute (compare to the estimate (4.9)) the Crank-Nicolson approximations W^n, $n = 1, \ldots, N$, which are defined by the numerical scheme (4.13) and the corresponding Crank-Nicolson reconstruction. However, it is noteworthy that in order to compute the approximations W^n, $n = 1, \ldots, N$, in the fully discrete case, we have to solve a linear system with the *same* matrix as in the case of the computation of the Crank-Nicolson approximations U^n, $n = 1, \ldots, N$, given by the numerical scheme (2.1). Thus, the extra cost is that at every time step n, we have to solve two linear systems with the same matrix, instead of one, in order to compute W^n. The numerical investigation of estimates (4.30) and (4.9) in fully discrete cases is an interesting problem and will be the subject of a forthcoming paper.

4.3. **An interesting special case**

In this subsection we consider the special case of problem (1.1) in which $f \equiv 0$ and $g = g(x)$ and we rewrite the theorems related to the $L^\infty(H^1)$ *a posteriori* error bounds pointing out the simplifications that can be done.

To this end, let $\{U^n\}_{n=0}^N$ be the Crank-Nicolson approximations given by

$$\begin{cases} \bar\partial U^n + \mathrm{i}(-\alpha\Delta + g)U^{n-\frac12} = 0, \quad n = 1,\dots,N, \\ U^0 = u_0 \quad \text{in } \bar\Omega, \end{cases} \tag{4.36}$$

and $U : [0,T] \to H_0^1(\Omega)$ the piecewise linear Crank-Nicolson approximation. Let also $\hat U : [0,T] \to H_0^1(\Omega)$ be the Crank-Nicolson reconstruction of U and $\hat r : [0,T] \to L^2(\Omega)$ the residual of $\hat U$. In particular, in this special case, we have that $G_U = gU$ (see (2.4)) and therefore the residual $\hat r$ is simply written as

$$\hat r(t) = \mathrm{i}(-\alpha\Delta + g)\left(\hat U - U\right)(t), \quad t \in I_n.$$

As in the previous subsection, let us consider the problem

$$\begin{cases} w_t - \mathrm{i}\alpha\Delta w + \mathrm{i}g(x)w = 0 & \text{in } \bar\Omega \times [0,T], \\ w = 0 & \text{on } \partial\Omega \times [0,T], \\ w(\cdot,0) = \mathrm{i}(\alpha\Delta - g)u_0 & \text{in } \bar\Omega. \end{cases} \tag{4.37}$$

Notice that since $g \in C^1(\bar\Omega)$ and $u_0, \Delta u_0 \in H_0^1(\Omega)$, the solution w of problem (4.37) is u_t, $w = u_t$, and not just an approximation of it.

Let W^n, $n = 1,\dots,N$, be the Crank-Nicolson approximations for problem (4.37) given by

$$\begin{cases} \bar\partial W^n + \mathrm{i}(-\alpha\Delta + g)W^{n-\frac12} = 0, \quad n = 1,\dots,N, \\ W^0 = \mathrm{i}(\alpha\Delta - g)u_0 \quad \text{in } \bar\Omega, \end{cases} \tag{4.38}$$

and $W : [0,T] \to H_0^1(\Omega)$ the linear Crank-Nicolson approximation corresponding to approximations $\{W^n\}_{n=0}^N$. Finally, let $\hat W : [0,T] \to H_0^1(\Omega)$ be the Crank-Nicolson reconstruction of W and $\hat R : [0,T] \to L^2(\Omega)$ the corresponding residual.

Proposition 4.2. *Let $\{U^n\}_{n=0}^N$ and $\{W^n\}_{n=0}^N$ be the Crank-Nicolson approximations* (4.36) *and* (4.38)*, respectively. Then, for $n = 0,1,\dots,N$,*

$$W^n = \mathrm{i}(\alpha\Delta - g)U^n. \tag{4.39}$$

Proof. Equality (4.39) can be proven by induction. Indeed, for $n = 0$, (4.39) is obvious. Let us suppose now that

$$W^{n-1} = \mathrm{i}(\alpha\Delta - g)U^{n-1}.$$

Using the numerical schemes (4.36) and (4.38) and the fact that the operators $\left(I \pm \mathrm{i}\frac{k_n}{2}(-\alpha\Delta + g)\right)$ and $\mathrm{i}(\alpha\Delta - g)$ commute, we can easily see that

$$\begin{aligned} \left(I + \mathrm{i}\frac{k_n}{2}(-\alpha\Delta + g)\right) W^n &= \mathrm{i}(\alpha\Delta - g)\left(I - \mathrm{i}\frac{k_n}{2}(-\alpha\Delta + g)\right) U^{n-1} \\ &= \left(I + \mathrm{i}\frac{k_n}{2}(-\alpha\Delta + g)\right)(\mathrm{i}(\alpha\Delta - g)U^n), \end{aligned}$$

whence we conclude that $W^n = \mathrm{i}(\alpha\Delta - g)U^n$, because of the uniqueness of W^n, $n = 0,1,\dots,N$, and the proof is complete. □

Corollary 4.2. *For $t \in I_n$, $n = 1, \dots, N$, the following equalities are valid:*

$$W(t) = \mathrm{i}(\alpha\Delta - g)U(t), \tag{4.40}$$

$$\hat{W}(t) = \mathrm{i}(\alpha\Delta - g)\hat{U}(t), \tag{4.41}$$

and

$$\hat{R}(t) = (-\alpha\Delta + g)^2 \left(\hat{U} - U\right)(t). \tag{4.42}$$

Corollary 4.3 (suboptimal *a posteriori* estimate)**.** *With the notation of this subsection, the following* a posteriori *estimate is valid, for $n = 1, \dots, N$,*

$$\max_{0\le t\le t^n} \left\| \left(u - \hat{U}\right)_t (t) \right\|_{L^2(\Omega)} \le \int_0^{t^n} \|(-\alpha\Delta + g)\left(\hat{U} - U\right)_t (t)\|_{L^2(\Omega)}\, \mathrm{d}t. \tag{4.43}$$

Remark 4.5. In this special case, $\hat{U}_t$ is a continuous function and thus the discontinuities that appear in estimate (4.9) do not appear in estimate (4.43).

Corollary 4.4 (recovery of optimality)**.** *With the notation of this subsection, the following estimate holds, for $n = 1, \dots, N$,*

$$\begin{aligned} \max_{0\le t\le t^n} \left\| \left(u - \hat{U}\right)_t (t) \right\|_{L^2(\Omega)} \le & \int_0^{t^n} \left\|(-\alpha\Delta + g)^2 \left(\hat{U} - U\right)(t)\right\|_{L^2(\Omega)} \mathrm{d}t \\ & + \max_{0\le t\le t^n} \left\|(-\alpha\Delta + g)\left(\hat{U} - U\right)(t)\right\|_{L^2(\Omega)}. \end{aligned} \tag{4.44}$$

Remark 4.6. A very interesting remark is that in this special case, there is no need to solve another linear system at each time step n in order to compute the approximations W^n. Indeed, because of Proposition 4.2, the Crank-Nicolson approximations $\{W^n\}_{n=0}^N$, the linear Crank-Nicolson approximation W and the Crank-Nicolson reconstruction $\hat{W}$ do not appear in the final estimate (4.43). Also, if we compare estimates (4.43) and (4.44), it becomes clear why estimate (4.44) is of optimal order of accuracy, while (4.43) is not. In (4.43), because we use $\hat{U}_t$ directly, we also have to use U_t which does not approximate u_t with optimal order. On the other hand, in estimate (4.44), instead of using $\hat{U}_t$ directly, we use $\mathrm{i}(\alpha\Delta - g)\hat{U}$ which is an optimal order approximation of it. This is the reason why the quantity $\max_{0\le t\le t^n} \|(-\alpha\Delta + g)(\hat{U} - U)(t)\|_{L^2(\Omega)} = \max_{0\le t\le t^n} \|\hat{r}(t)\|_{L^2(\Omega)}$ appears on the right hand site of estimate (4.44). Moreover, in this way, we avoid using U_t, but we use $\mathrm{i}(\alpha\Delta - g)U$ instead, which is an optimal order approximation to $\mathrm{i}(\alpha\Delta - g)u$.

Combining the estimate (4.10) (or (4.31)) firstly with (4.43) and then with (4.44) we immediately conclude to:

Corollary 4.5. (*a posteriori* estimates in the $L^\infty(H^1)$-norm). *With the notation of the previous corollaries, the following* a posteriori *error estimates are valid, for $n = 1, \dots, N$,*

$$\begin{aligned} \max_{0\le t\le t^n} \left\|\nabla\left(u - \hat{U}\right)(t)\right\|^2_{L^2(\Omega)} \le & \frac{2}{\alpha}(t^n \sup_{x\in\Omega} |g(x)| + 1) \\ & \times \int_0^{t^n} \left\|(-\alpha\Delta + g)\left(\hat{U} - U\right)(t)\right\|_{L^2(\Omega)} \mathrm{d}t \\ & \times \int_0^{t^n} \left\|(-\alpha\Delta + g)\left(\hat{U} - U\right)_t (t)\right\|_{L^2(\Omega)} \mathrm{d}t, \end{aligned} \tag{4.45}$$

and

$$\max_{0\le t\le t^n}\left\|\nabla\left(u-\hat U\right)(t)\right\|^2_{L^2(\Omega)} \le \frac{2}{\alpha}(t^n\sup_{x\in\Omega}|g(x)|+1) \times\int_0^{t^n}\left\|(-\alpha\Delta+g)\left(\hat U-U\right)(t)\right\|_{L^2(\Omega)}\mathrm{d}t \times\left[\int_0^{t^n}\left\|(-\alpha\Delta+g)^2\left(\hat U-U\right)(t)\right\|_{L^2(\Omega)}\mathrm{d}t + \max_{0\le t\le t^n}\left\|(-\alpha\Delta+g)\left(\hat U-U\right)(t)\right\|_{L^2(\Omega)}\right]. \tag{4.46}$$

5. Numerical experiments

In this section we verify numerically the theory of Sections 3 and 4. We consider two simple, one-dimensional, model problems related to the equation

$$u_t-\mathrm{i}\frac{\varepsilon}{2}u_{xx}+\frac{\mathrm{i}}{\varepsilon}V(x)u=0. \tag{5.1}$$

In particular, as a first model problem, we consider the free Schrödinger equation; in this case $V\equiv 0$, with $\varepsilon=0.2$. For the second numerical experiment we take the harmonic oscillator $V(x)=\frac{x^2}{32}$ and $\varepsilon=1$. In both cases we take as initial value

$$u_0(x)=\mathrm{e}^{-\frac{x^2}{2}+\mathrm{i}\frac{x^2}{2\varepsilon}}. \tag{5.2}$$

We consider problem (5.1)–(5.2) in $\bar\Omega\times[0,T]=[-8,8]\times[0,1]$ and we discretize it in space by smooth periodic splines of degree 6 and in time by the Crank-Nicolson method. Notice that, since we consider (5.2) in $[-8,8]$, we have that u_0 is numerically zero at the boundary. This makes our theory applicable.

In order to overkill the error due to the space discretization, and therefore be able to check the behaviour of time error estimators presented in Sections 3 and 4, we consider a very fine mesh size. In particular we take $h=\frac{1}{60}$. This is indeed a very fine mesh size, if we take into account that the data are smooth for both model problems, and thus we implement by a method of order 7 in space.

Let us denote by E the $L^\infty(L^2)$ *a posteriori* error estimator (*cf.* (3.2)), and by E_1 and E_2 the *a posteriori* error estimators appearing in estimates (4.43) and (4.44), respectively. We set $c:=\frac{4}{\varepsilon}(\sup_{x\in[-8,8]}|V(x)|+1)$ and we define $\mathcal{E}_1$ and $\mathcal{E}_2$ to be the $L^\infty(H^1)$ error estimators discussed in Section 4, *i.e.*, we define

$$\mathcal{E}_1:=\sqrt{cEE_1}\ \text{ and }\ \mathcal{E}_2:=\sqrt{cEE_2},$$

cf. (4.45) and (4.46). Clearly the difference between estimators $\mathcal{E}_1$ and $\mathcal{E}_2$ is that estimator E_1 in $\mathcal{E}_1$ is replaced by E_2 in $\mathcal{E}_2$. In Tables 1–6 we present numerical evidence that the error estimators E and E_2 (and thus $\mathcal{E}_2$) are of second order of accuracy, while E_1 is of first order (and thus $\mathcal{E}_1$ is of order $\frac{3}{2}$). Since we are mainly interested in verifying the order of the estimators, we implement with various constant time steps.

We also study the efficiency of the estimators by comparing them with a reference error. More precisely, we approximated the exact $L^\infty(L^2)$ and $L^\infty(H^1)$ error as follows: We computed a reference solution u_{ref} obtained by discretizing with a very fine time step (we took $k^{-1}=20\,480$) and we calculated

$$\mathrm{Eref}_1:=\max_{0\le n\le N}\|u_{\mathrm{ref}}(t^n)-U^n\|_{L^2(-8,8)},$$

and

$$\mathrm{Eref}_2:=\max_{0\le n\le N}\|\nabla u_{\mathrm{ref}}(t^n)-\nabla U^n\|_{L^2(-8,8)},$$

as approximations to the exact errors. With respect to the reference error Eref_1 the effectivity index ei of the estimator E is defined as

$$ei:=\frac{E}{\mathrm{Eref}_1}\cdot$$

TABLE 1. $L^\infty(L^2)$ reference error and estimator for the free Schrödinger equation and the corresponding effectivity index.

k^{-1}	Eref_1	E	ei
10	1.4573 e−01	1.9571 e−01	1.3430
20	5.2215 e−02	5.7824 e−02	1.1074
40	1.4920 e−02	1.5377 e−02	1.0306
80	3.8499 e−03	3.9145 e−03	1.0168
160	9.6877 e−04	9.8329 e−04	1.0150
320	2.4251 e−04	2.4612 e−04	1.0149
640	6.0605 e−05	6.1549 e−05	1.0156
1280	1.5108 e−05	1.5388 e−05	1.0185

TABLE 2. Estimators E_1 and E_2 and orders of convergence in the case of the free Schrödinger equation.

k^{-1}	E_1	Order	E_2	Order
10	11.743	–	3.6511	–
20	6.9389	0.75902	1.1522	1.6639
40	3.6904	0.91093	3.1641 e−01	1.8645
80	1.8789	0.97389	8.1429 e−02	1.9582
160	9.4396 e−01	0.99309	2.0516 e−02	1.9888
320	4.7255 e−01	0.99825	5.1393 e−03	1.9971
640	2.3634 e−01	0.99960	1.2855 e−03	1.9992
1280	1.1818 e−01	0.99988	3.2141 e−04	1.9998

TABLE 3. $L^\infty(H^1)$ reference error, suboptimal and optimal estimators, and the corresponding effectivity indices for the free Schrödinger equation.

k^{-1}	Eref_2	$\mathcal{E}_1$	ei_1	$\mathcal{E}_2$	ei_2
10	1.5817	6.7796	4.2863	3.7804	2.3901
20	6.3194 e−01	2.8328	4.4827	1.1543	1.8266
40	1.9064 e−01	1.0653	5.5880	3.1193 e−01	1.6362
80	4.9890 e−02	3.8354 e−01	7.6877	7.9844 e−02	1.6004
160	1.2586 e−02	1.3625 e−01	10.825	2.0087 e−02	1.5960
320	3.1522 e−03	4.8229 e−02	15.300	5.0297 e−03	1.5956
640	7.8784 e−04	1.7057 e−02	21.650	1.2579 e−03	1.5966
1280	1.9641 e−04	6.0310 e−03	30.706	3.1451 e−04	1.6013

Similarly, with respect to Eref_2, the effectivity indices ei_1 and ei_2 of estimators $\mathcal{E}_1$ and $\mathcal{E}_2$, are

$$ei_1 := \frac{\mathcal{E}_1}{\text{Eref}_2} \quad \text{and} \quad ei_2 := \frac{\mathcal{E}_2}{\text{Eref}_2},$$

respectively. We compute ei and ei_1, ei_2 in Tables 1 and 3 for the case of free Schrödinger equation, and in Tables 4 and 6 for the case of the harmonic oscillator.

TABLE 4. $L^\infty(L^2)$ reference error and estimator for the harmonic oscillator and the corresponding effectivity index.

k^{-1}	Eref_1	E	ei
5	4.5504 e−02	4.8881 e−02	1.0742
10	1.3592 e−02	1.3880 e−02	1.0212
20	3.5905 e−03	3.6216 e−03	1.0087
40	9.1041 e−04	9.1628 e−04	1.0064
80	3.8499 e−04	2.2978 e−04	1.0060
160	5.7148 e−05	5.7490 e−05	1.0060
320	1.4287 e−05	1.4375 e−05	1.0062
640	3.5695 e−06	3.5940 e−06	1.0069
1280	8.8976 e−07	8.9851 e−07	1.0098

TABLE 5. Estimators E_1 and E_2 and orders of convergence in the case of the harmonic oscillator.

k^{-1}	E_1	Order	E_2	Order
5	1.4664	–	4.2230 e−01	–
10	8.3283 e−01	0.81618	1.3022 e−01	1.6973
20	4.3460 e−01	0.93833	3.9468 e−02	1.7222
40	2.1991 e−01	0.98277	1.1183 e−02	1.8193
80	1.1029 e−01	0.99561	2.9104 e−03	1.9420
160	5.5190 e−02	0.99882	7.3542 e−04	1.9846
320	2.7600 e−02	0.99973	1.8441 e−04	1.9956
640	1.3801 e−02	0.99989	4.6287 e−05	1.9942
1280	6.9005 e−03	1.0000	1.2507 e−05	1.8879

TABLE 6. $L^\infty(H^1)$ reference error, suboptimal and optimal estimators, and the corresponding effectivity indices for the harmonic oscillator.

k^{-1}	Eref_2	$\mathcal{E}_1$	ei_1	$\mathcal{E}_2$	ei_2
5	1.4366 e−01	9.2746 e−01	6.4559	4.9770 e−01	3.4644
10	4.4920 e−02	3.7245 e−01	8.2914	1.4728 e−01	3.2787
20	1.2042 e−02	1.3743 e−01	11.412	4.1416 e−02	3.4393
40	3.0642 e−03	4.9173 e−02	16.048	1.1089 e−02	3.6189
80	7.6936 e−04	1.7439 e−02	22.667	2.8329 e−03	3.6821
160	1.9254 e−04	6.1705 e−03	32.048	7.1229 e−04	3.6994
320	4.8138 e−05	2.1820 e−03	45.328	1.7835 e−04	3.7050
640	1.2026 e−05	7.7150 e−04	64.153	4.4679 e−05	3.7152
1280	2.9981 e−06	2.7276 e−04	90.978	1.1612 e−05	3.8731

Observations. From Tables 1 and 4 we conclude the optimality of the $L^\infty(L^2)$ *a posteriori* error estimator E. Indeed, in both cases the effectivity index ei is almost constant; it is around 1.01 and 1.006 for the free Schrödinger equation and the harmonic oscillator, respectively. Similarly, Tables 3 and 6 indicate the efficiency of the $L^\infty(H^1)$ *a posteriori* error estimator $\mathcal{E}_2$. The effectivity index ei_2 is almost constant and around 1.60 for the free Schrödinger equation, and around 3.70 for the harmonic oscillator. The fact that ei_1 grows while the time step reduces, proves that the $L^\infty(H^1)$ estimator $\mathcal{E}_1$ does not behave asymptotically as the reference $L^\infty(H^1)$-error; in particular it proves that $\mathcal{E}_1$ is not of optimal order of accuracy. This is also clear from Tables 2 and 5: The estimator E_1 which is part of $\mathcal{E}_1$ is of first, instead of second order of accuracy. On the other hand, in both examples, E_2 is of optimal second order.

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