ERROR CONTROL FOR TIME-SPLITTING SPECTRAL APPROXIMATIONS OF THE SEMICLASSICAL SCHRÖDINGER EQUATION

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Abstract. We prove a posteriori error estimates of optimal order in the $L^\infty(L^2)$-norm for time-splitting spectral methods applied to the linear Schrödinger equation in the semiclassical regime.

The a posteriori error estimates are obtained by considering an appropriate extension in time of the numerical schemes and using energy techniques. Numerical experiments are presented which confirm our theoretical results.

1. Introduction

The solution of the Schrödinger equation

$$\varepsilon u_\varepsilon^t - \frac{i}{2} \Delta u_\varepsilon + i V(x) u_\varepsilon = 0, \quad x \in \mathbb{R}^d, \quad t \in \mathbb{R},$$

with high frequency initial data

$$u_\varepsilon(x, 0) = u_\varepsilon^0(x), \quad x \in \mathbb{R}^d,$$

in the semiclassical regime $(0 < \varepsilon \ll 1)$ is an important and challenging problem. In solid state physics, $\varepsilon$ is the scaled Planck constant and $V(x)$ is a smooth electrostatic potential. The wave function $u_\varepsilon(x, t)$ is used to define primary physical quantities, usually referred to as observables (see, e.g., [6, 1]), such as the position density and the current density:

$$n_\varepsilon(x, t) = |u_\varepsilon(x, t)|^2,$$

$$J_\varepsilon(x, t) = \varepsilon \text{Im}(\overline{u_\varepsilon(x, t)} \nabla u_\varepsilon(x, t)).$$

It is known that when $\varepsilon$ is small, the wave function $u_\varepsilon(x, t)$ and the related observables become oscillatory of wave length $O(\varepsilon)$. The numerical resolution of (1.1) is quite hard. Direct discretization methods of (1.1) resolve satisfactorily the wave function only for small mesh sizes compared to $\varepsilon$, [10, 1, 11]. In [10] for finite differences, and in [1] for spectral splitting methods, sharp conditions of asymptotic nature on the behavior of the spatial mesh size $h$ and the time step $k$ as functions of $\varepsilon$ are given in order to have satisfactorily approximations of the wave function and of the observables. It turns out that these conditions are less stringent in the case of the spectral splitting methods [1] and, indeed, numerical evidence and Wigner type techniques lead to the conclusion that $k$ may be chosen independently of $\varepsilon$, while a weak condition of the form $h = O(\varepsilon)$ is needed to obtain reasonably good approximations of the observables.

In this paper we focus on the spectral splitting methods of Bao, Jin and Markowich [1]. Our aim is to provide an error control of a posteriori type for these approximations of the semiclassical Schrödinger equation. In fact, our results permit a direct assessment of the quality of approximation without having additional (not known in real applications) information on the exact solution. In the present paper we have focused on the approximation of the wave function itself. The question of a posteriori “error assessment” of the observables will be the subject of a forthcoming paper.

In Section 3 we prove an estimate of the type (Theorem 3.1)

$$\max_{0 \leq t \leq T} \|u_\varepsilon^t(t) - U^T_I(t)\|_{L^2(a,b)} \leq \mathcal{E}(U^T_I, u_\varepsilon^0, V),$$

Date: December 20, 2009.

Key words and phrases. Schrödinger equation, time-splitting spectral methods, a posteriori estimates.

The research of I. K. and Ch. M. was supported in part by the the European Union grant No. MEST-CT-2005-021122 (Differential Equations with Applications in Science and Engineering). I. K. acknowledges support by the “Alexander S. Onassis Public Benefit Foundation” and “The A. G. Leventis Foundation”. 

1
where $U^\varepsilon_j$ is an appropriate continuous extension of the spectral-splitting approximation and $\mathcal{E}(U^\varepsilon_j, u_0^\varepsilon, V)$ is an a posteriori estimator that depends on the computed approximation only and the data. The need of the intermediate function $U^\varepsilon_j$ and the derivation of the basic estimate follows, in principle, the approach in [9]. Section 3 is devoted to the proof of (1.5) and to a detailed analysis that verifies the correct asymptotic behavior of the estimator under reasonable assumptions on the mesh, the potential and the initial value (Corollary 3.1) in the case of the Lie splitting spectral method. Our results deal with the case of non-constant potentials, for if $V$ is constant the estimators vanish as expected. Similar results are shown in Section 5 for the Strang splitting method, see Theorem 5.1. Notice, however, that the right definition of the continuous extension $U^\varepsilon_j$ is more involved in this case. Section 4 is devoted to the proof of Proposition 3.1 which is a stability result for the discrete solution. In Section 6 we report on the outcome of numerical experiments performed with the two methods and computationally evaluate the behavior of the estimators. The numerical tests confirm the correct order of the estimators and the fact that $\mathcal{E}(U^\varepsilon_j, u_0^\varepsilon, V)$ provides an accurate assessment on the behavior of the error, using only information on the already computed solution.

2. Preliminaries

For the sake of clarity and the simplicity of the notation in the analysis below we shall consider the one dimensional case ($d = 1$). However, we can easily extend our results to higher dimensions by considering tensor product grids. We shall be concerned with the numerical approximation of problem (1.1)–(1.2) with periodic boundary conditions:

\begin{equation}
\varepsilon u_1^\varepsilon - \frac{\varepsilon^2}{2}u_{1xx} + iV(x)u_1^\varepsilon = 0, \quad a < x < b, \quad 0 < t \leq T,
\end{equation}

\begin{equation}
u^\varepsilon(x,0) = u_0^\varepsilon(x), \quad a \leq x \leq b
\end{equation}

\begin{equation}u^\varepsilon(a,t) = u^\varepsilon(b,t), \quad u_1^\varepsilon(a,t) = u_1^\varepsilon(b,t), \quad 0 < t \leq T.
\end{equation}

For $M \in \mathbb{N}$ even, let $x_j = a + jh$, $j = 0, 1, \ldots, M$, denote the grid points of a uniform partition of $[a, b]$ of size $h = (b - a)/M$. We let $0 = t^0 < t^1 < \cdots < t^{N} = T$ be a partition of $[0, T]$, and

$$k_n = t^{n+1} - t^n, \quad k = \max_{0 \leq n \leq N-1} k_n.$$

For $j = 0, 1, \ldots, M - 1$ and $n = 0, \ldots, N$, let $U_j^{\varepsilon,n}$ be approximations to the values $u^\varepsilon(x_j, t^n)$ of the exact solution $u^\varepsilon$. The main idea of the Lie splitting spectral method is to split equation (2.1) into two simpler equations

\begin{equation}\varepsilon u_{11}^\varepsilon - \frac{\varepsilon^2}{2}u_{11xx} = 0
\end{equation}

and

\begin{equation}\varepsilon u_{22}^\varepsilon + iV(x)u_2^\varepsilon = 0.
\end{equation}

Let us suppose that for $x \in [a, b]$, we have an approximation $U^\varepsilon_n(x)$ to the exact solution $u^\varepsilon(x, t^n)$. Then, from time $t = t^n$ to time $t = t^{n+1}$, equation (2.4) will be discretized in space by the spectral method and then integrated in time exactly with initial value $U^\varepsilon_n(x)$. Finally, (2.5) will be solved exactly in $(t^n, t^{n+1})$ with the approximate solution of (2.4) at the node $t = t^{n+1}$ as initial value at $t^n$. The Lie time-splitting spectral method is defined as

\begin{equation}U_j^{\varepsilon,0} = u_0^\varepsilon(x_j), \quad j = 0, 1, \ldots, M - 1,
\end{equation}

\begin{equation}U_j^{\varepsilon,\varepsilon} = \frac{1}{M} \sum_{\ell = -M/2}^{M/2 - 1} e^{-i\ell a} \mu_{\ell} u_{\ell}^{\varepsilon} e^{i\mu_{\ell}(x_j - a)}, \quad j = 0, 1, \ldots, M - 1,
\end{equation}

\begin{equation}U_j^{\varepsilon,n+1} = e^{-iV(x_j)k_n} U_j^{\varepsilon,n}, \quad j = 0, 1, \ldots, M - 1,
\end{equation}

where $U_j^{\varepsilon,n}$ are defined by

\begin{equation}\mu_{\ell} = \frac{2\pi \ell}{b - a}, \quad U_j^{\varepsilon,n} = \sum_{j = 0}^{M-1} U_j^{\varepsilon,n} e^{-i\mu_{\ell}(x_j - a)}, \quad \ell = -M/2, \ldots, M/2 - 1.
\end{equation}
In the sequel we shall denote by $U_j^{\varepsilon,n}$ the Lie time-splitting trigonometric spectral approximations at the nodes $t^n$, i.e.,

$$U_j^{\varepsilon,n}(x) = \frac{1}{M} \sum_{\ell=-M/2}^{M/2-1} \hat{U}_\ell^{\varepsilon,n} e^{i\mu_\ell (x-a)}.$$  

(2.10)

It is known that the time discretization error of the Lie time-splitting spectral method is of first order in $k$ for any fixed $\varepsilon > 0$, see, e.g., [2]. We shall also consider and analyze the so-called Strang splitting spectral method which achieves second order accuracy in time. For the sake of clarity of the exposition we defer the introduction of the method until Section 5. Details on the derivation of the two methods and a priori error analysis may be found in [1].

We shall make frequent use of the following trigonometric interpolation operator: Let

$$V_h = \text{span} \{e^{i\mu_\ell (x-a)} : -M/2 \leq \ell \leq M/2 - 1, x \in [a,b] \}$$

denote the space of trigonometric polynomials of degree at most $M/2$ and define $T : C[a,b] \to V_h$ by

$$(Tf)(x) = \frac{1}{M} \sum_{\ell=-M/2}^{M/2-1} \hat{f}_\ell e^{i\mu_\ell (x-a)},$$

where $\hat{f}_\ell$ denote the discrete Fourier coefficients of $f$, i.e.,

$$\hat{f}_\ell = \sum_{j=0}^{M-1} f(x_j) e^{-i\mu_\ell (x_j-a)}, \quad \ell = -M/2, \ldots, M/2 - 1.$$  

(2.11)

The operator $T$ is obviously well defined and linear. An immediate consequence of its definition is the fact that $Tf$ interpolates $f$ at the grid points $x_j, j = 0, 1, \ldots, M-1$. In addition, $Tf = f$ for $f \in V_h$. It is also easy to check that $T$ commutes with differentiation with respect to time, but, in general, $Tf_x \neq (Tf)_x$.

A fundamental tool in the a posteriori error analysis is the introduction of a continuous and computable spectral approximation which coincides with the discrete spectral approximations produced by the Lie (or Strang) method at the time nodes $t^n, n = 0, 1, \ldots, N$. The continuous Lie splitting approximation $U_j^\varepsilon : [a,b] \times [0,T] \to \mathbb{C}$ is constructed as follows: First, we let

$$U^\varepsilon(x,0) = u_0^\varepsilon(x), \quad x \in [a,b].$$

For $n = 0, 1, \ldots, N-1$, $t \in (t^n, t^{n+1}]$ and $x \in [a,b]$ we define, cf. (2.7)–(2.8),

$$U_j^\varepsilon(x,t) = \frac{1}{M} \sum_{\ell=-M/2}^{M/2-1} e^{-i\mu_\ell \int_0^t V(x,s) ds} \hat{U}_\ell^{\varepsilon,n} e^{i\mu_\ell (x-a)},$$

(2.13)

$$U^\varepsilon(x,t) = e^{-iV(x,t)} U_j^\varepsilon(x,t),$$

(2.14)

where the Fourier coefficients $\hat{U}_\ell^{\varepsilon,n}$ are defined as in (2.9). Next, we define the time-continuous discrete Fourier coefficients $\hat{U}_\ell^\varepsilon$ are defined as in (2.9). Next, we define the time-continuous discrete Fourier coefficients

$$\hat{U}_\ell^{\varepsilon,n}(t) = \sum_{j=0}^{M-1} U_j^{\varepsilon}(x_j,t) e^{-i\mu_\ell (x_j-a)}, \quad \ell = -M/2, \ldots, M/2 - 1,$$

and, finally,

$$U_j^\varepsilon(x,t) = \frac{1}{M} \sum_{\ell=-M/2}^{M/2-1} \hat{U}_\ell^{\varepsilon,n} e^{i\mu_\ell (x-a)}, \quad x \in [a,b], \quad t \in (t^n, t^{n+1}].$$  

(2.15)

(2.16)

It follows immediately from the definition of $U_j^\varepsilon$ that $U_j^\varepsilon(x,t^n) = U_j^{\varepsilon,n}(x)$, so that $U^\varepsilon$ coincides with the Lie time-splitting spectral approximations at the time nodes $t^n, n = 0, 1, \ldots, N$. To show that $U^\varepsilon \in C([a,b] \times [0,T])$ it is enough to prove that

$$\lim_{t \to t^n+} \hat{U}_\ell^\varepsilon(t^n) = \hat{U}_\ell^\varepsilon(t^n) \quad \text{or} \quad \lim_{t \to t^{n+}} U_j^\varepsilon(x,t) = U_j^{\varepsilon,n},$$

for all $\ell, j$.
where \( U_{j}^{n,m} \) are the approximations produced by the Lie splitting spectral method (2.6)–(2.8). Either of these relations may be easily verified using the fact that

\[
\sum_{\ell = -M/2}^{M/2 - 1} e^{i2\pi(j_{1}-j_{2})\ell} = \begin{cases} M & \text{if } j_{1} - j_{2} = sM, \\ 0 & \text{if } j_{1} - j_{2} \neq sM, \end{cases}
\]

where \( s \) is an integer. Obviously, \( U_{\varepsilon}^{n+\dagger} \) and \( U_{\varepsilon}^{n} \) belong to the space \( C^{\infty,\infty}([a,b] \times (t^{n},t^{n+1})) \) and thus \( U_{\varepsilon}^{n+\dagger} \) belongs to the same space.

The final ingredient needed in the a posteriori error analysis of the next section is the residual \( R_{\varepsilon} : [a,b] \times (t^{n},t^{n+1}) \rightarrow \mathbb{C} \),

\[
R_{\varepsilon}(x,t) = \varepsilon U_{j,l}^{n}(x,t) - \frac{i}{2} U_{j,xx}^{n}(x,t) + iV(x)U_{j}^{n}(x,t),
\]

i.e., the amount by which the continuous Lie splitting approximation \( U_{j}^{n} \) misses to satisfy (2.1).

Let \( \varepsilon \) be the solution of problem (2.1)–(2.3) and \( U_{j}^{n} \) the continuous Lie splitting approximation (2.16). We assume that \( u_{0j}^{n} \in L^{2}(a,b) \) and \( V \in L^{\infty} \). Then, for \( n = 0,1,\ldots,N-1 \), we have

\[
\max_{0 \leq t \leq t^{n+1}} \| u_{j}^{n}(t) - U_{j}^{n}(t) \|_{L^{2}(a,b)} \leq \| u_{0j}^{n} - Tu_{0j}^{n} \|_{L^{2}(a,b)} + \sum_{k=0}^{n} \int_{t^{k}}^{t^{k+1}} \frac{1}{\varepsilon} \| R_{\varepsilon}(t) \|_{L^{2}(a,b)} dt,
\]

where \( R_{\varepsilon} \) is the a posteriori quantity given in (2.18).

**Proof.** Let \( \varepsilon = u - U_{j}^{n} \) be the error. Then for \( n = 0,1,\ldots,N-1 \), \( \varepsilon \) satisfies the initial and boundary value problem

\[
\begin{align*}
\varepsilon \varepsilon_{t}^{n} - \frac{i}{2} \varepsilon_{xx}^{n} + i V(x)\varepsilon^{n} &= -R_{\varepsilon}^{n} & \text{in } [a,b] \times (t^{n},t^{n+1}), \\
\varepsilon^{n}(&a,\cdot) = \varepsilon_{x}^{n} & \text{in } [a,b], \\
\varepsilon^{n}(a,\cdot) = \varepsilon^{n}(b,\cdot) & \text{in } (t^{n},t^{n+1}),
\end{align*}
\]

with \( \varepsilon_{0j}^{n} = u_{0j}^{n} - Tu_{0j}^{n} \) in \([a,b]\). Taking in the first equation of (3.2) the \( L^{2}\)-inner product with \( \varepsilon \) and then real parts we conclude, for \( m = 0,1,\ldots,n \), that

\[
\frac{d}{dt} \| \varepsilon^{n}(t) \|_{L^{2}(a,b)} \leq \frac{1}{\varepsilon} \| R_{\varepsilon}(t) \|_{L^{2}(a,b)}, \quad t \in (t^{m},t^{m+1}).
\]

Integrating (3.3) from \( t^{m} \) to \( t \in (t^{m},t^{m+1}) \), we end up with

\[
\| \varepsilon^{n}(t) \|_{L^{2}(a,b)} \leq \| \varepsilon^{n}(t^{m}) \|_{L^{2}(a,b)} + \int_{t^{m}}^{t} \frac{1}{\varepsilon} \| R_{\varepsilon}(t) \|_{L^{2}(a,b)} dt.
\]

Since \( \| \varepsilon(t) \|_{L^{2}(a,b)} \) is continuous in \([0,t^{n+1}]\), summing up relations (3.4) over \( m \), we conclude the a posteriori error estimate (3.1).

**Remark 3.1.** \( R_{\varepsilon} \) is a computable quantity and its calculation can be implemented by using its equivalent expression (3.11).
Our next task is to verify that the estimator in Theorem 3.1 is of optimal order. We address this issue both numerically and theoretically. In Section 6 we show for potentials that are used in the wave propagation community (c.f. [1], [3], [8] [13], [14]), that indeed the estimator has the right order. In the remaining part of this section we focus on proving that the estimator is of optimal order in the case where the potential is smooth enough. As a consequence, we provide an alternative “a posteriori” proof of the convergence rate of the method to the one discussed in [1].

To this end, we shall assume for the remaining part of this section that the initial condition $u_0$ and the electrostatic potential $V$ are $C^\infty$ on $\mathbb{R}$ and $(b-a)$-periodic. Further, we shall assume that for $m \in \mathbb{N}_0$ there exist positive constants $A_m$ and $B_m$ of $\varepsilon$ (and of course independent of the time and the space steps) such that

$$(3.5) \quad \|\frac{d^m}{dx^m}u_0\|_{L^2(a,b)} \leq \frac{A_m}{\varepsilon^m}$$

$$(3.6) \quad \|\frac{d^m}{dx^m}V\|_{L^\infty(a,b)} \leq B_m.$$  

For example, assumption (3.5) is satisfied if $u_0$ is the semiclassical WKB initial data

$$(3.7) \quad u_0(x) = \sqrt{n_0(x)} e^{iS_0(x)/\varepsilon}, \quad x \in \mathbb{R},$$

where $n_0$ and $S_0$ are real, $C^\infty$ on $\mathbb{R}$ and $(b-a)$-periodic. Furthermore, $n_0$ is positive and bounded away from 0. In the analysis below, we will need the following proposition.

**Proposition 3.1.** Let the potential $V$ be $C^\infty$ and $(b-a)-$periodic and assume that (3.5) and (3.6) are valid. Then for $m \in \mathbb{N}_0$, there exist positive constants $C_m$, which remain bounded while $\varepsilon$ tends to zero, and are independent of time and space steps, such that

$$(3.8) \quad \max_{0 \leq n \leq N} \|\frac{d^m}{dx^m}U^\varepsilon,n\|_{L^2(a,b)} \leq C_m \varepsilon^m.$$  

We postpone the proof of Proposition 3.1 until the next section. We just mention here that the proof of Proposition 3.1 is technical and uses stability arguments for the numerical scheme (2.6)–(2.10).

Our final assumption is the mesh condition

$$(3.9) \quad \frac{h}{\varepsilon(b-a)} = O(1).$$  

**Estimation of the residual.** Using the definition of the residual, the fact that

$$(3.10) \quad U^\varepsilon_t(x,t) = T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t), \quad x \in [a,b], \quad t \in [0,T],$$

and the properties of the trigonometric interpolant, we obtain for $t \in (t^n,t^{n+1})$, $n = 0, 1, \ldots, N-1$, and $x \in [a,b]$ that

$$(3.11) \quad R^\varepsilon(x,t) = \varepsilon \left[ T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t) \right]_x - \frac{\varepsilon^2}{2} \left[ T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t) \right]_{xx}$$

$$\quad + iV(x) T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t))$$

$$\quad - iV(x) T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t)) + \varepsilon T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t))$$

$$\quad - i\varepsilon^2 \left[ T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t) \right]_{xx} + iV(x) T(e^{-iV(x)\frac{t-n}{\varepsilon}} U^\varepsilon,*) (x,t).$$

**Remark 3.2.** If $V(x) \equiv V$ is a constant electrostatic potential, then for $n = 0, 1, \ldots, N-1$, $R^\varepsilon \equiv 0$ in $(t^n,t^{n+1})$. To see this, notice that from (3.11) we have

$$(3.12) \quad R^\varepsilon(x,t) = \varepsilon e^{-iV(x)\frac{t-n}{\varepsilon}} T(U^\varepsilon,*) (x,t) - \frac{\varepsilon^2}{2} e^{-iV(x)\frac{t-n}{\varepsilon}} [T(U^\varepsilon,*) (x,t)]_{xx},$$

because of the linearity of $T$. On the other hand, for every $t \in (t^n,t^{n+1})$, $n = 0, 1, \ldots, N-1$, we have $U^\varepsilon, \in V_h$. A straightforward calculation shows that

$$(3.13) \quad \varepsilon U^\varepsilon, - \frac{\varepsilon^2}{2} U^\varepsilon, xx = 0 \quad \text{in} \ [a,b] \times (t^n,t^{n+1}).$$
Therefore, since $T$ restricted on $V_h$ is the identity, we have
\[ R^*(x, t) = e^{-iV(x)} \left( e^{U^{\varepsilon, *}(x, t)} - \frac{i}{2} U^{\varepsilon, *}_{xx}(x, t) \right) = 0. \]

Henceforth we shall assume that $V(x)$ is a nonconstant electrostatic potential.

Combining (3.12) and (3.11) we conclude that
\begin{equation}
R^*(x, t) = i \left[ V(x) \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) - \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) \right] \nonumber
\end{equation}
\begin{equation}
+ \frac{i \varepsilon^2}{2} \left[ \left( e^{-iV(x)} \frac{\partial n}{\partial x} U^{\varepsilon, *}(x, t) \right) \right] xx. \nonumber
\end{equation}

We shall write,
\begin{equation}
R^*_c(x, t) = R^*_c(x, t) + R^*_c(x, t) + R^*_c(x, t) + R^*_c(x, t), \nonumber
\end{equation}
where
\begin{equation}
R^*_c(x, t) = i V(x) \left[ \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right] \nonumber
\end{equation}
\begin{equation}
R^*_c(x, t) = i \left[ V(x) \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) - \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) \right] \nonumber
\end{equation}
\begin{equation}
R^*_c(x, t) = i \frac{\varepsilon^2}{2} \left[ \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) \right] xx, \nonumber
\end{equation}
\begin{equation}
R^*_c(x, t) = i \frac{\varepsilon^2}{2} \left[ \left( e^{-iV(x)} \frac{\partial n}{\partial t} U^{\varepsilon, *}(x, t) \right) \right] xx. \nonumber
\end{equation}

We shall estimate each one of the above terms separately. Notice that all terms in $R^*_c$ involve differences of the form $v - V v$. The term $R^*_c$ is expected to represent the temporal error. To further estimate the terms in $R^*_c$ we shall need the following theorem, which is an immediate consequence of Theorem 3 of [12].

**Theorem 3.2.** Let $C^\infty_p([a, b])$ denote the set of infinitely differentiable on $\mathbb{R}$ and $(b-a)$-periodic functions. Also, let $m \in \mathbb{N}$ and $n \in \mathbb{N}_0$ with $n \leq m$. Then, there exists a constant $D > 0$, depending only on $b - a$, such that
\begin{equation}
\|\frac{d^n}{dx^n}(w - Tv)\|_{L^2([a, b])} \leq D (\frac{h}{b-a})^{m-n} \|\frac{d^n}{dx^n}w\|_{L^2([a, b])}, \quad \forall w \in C^\infty_p([a, b]). \nonumber
\end{equation}

**Proposition 3.2.** Under assumptions (3.5) and (3.6), it holds for $m \in \mathbb{N}_0$ that
\begin{equation}
\sup_{0 \leq t \leq T} \left| \frac{\partial^n}{\partial x^n} U^{\varepsilon, *}(t) \right|_{L^2([a, b])} \leq \frac{C_m}{\varepsilon^m}, \nonumber
\end{equation}
where $C_m$, $m \in \mathbb{N}_0$, are the constants in (3.8).

**Proof.** From (2.10), the definition of $U^{\varepsilon, *}$ and (3.12) we conclude that for $n = 0, 1, \ldots, N - 1$, $U^{\varepsilon, *}$ satisfies the initial and boundary value problem
\begin{equation}
U^{\varepsilon, *}_t \left( \frac{d^n}{dx^n} U^{\varepsilon, *}(t) \right) + \frac{\varepsilon^2}{2} U^{\varepsilon, *}_{xx} = 0 \quad \text{in } [a, b] \times (t^n, t^{n+1}), \nonumber
\end{equation}
with periodic boundary conditions. Therefore, for every $m \in \mathbb{N}_0$, 
\begin{equation}
\left( \frac{d^n}{dx^n} U^{\varepsilon, *}(t) \right) + \frac{\varepsilon^2}{2} \left( \frac{d^n}{dx^n} U^{\varepsilon, *}(t) \right)_{xx} = 0 \quad \text{in } [a, b] \times (t^n, t^{n+1}). \nonumber
\end{equation}
Taking in the above relation the $L^2$-inner product with $\frac{d^n}{dx^n} U^{\varepsilon, *}$ and then real parts we conclude, for $n = 0, 1, \ldots, N - 1$ and $t \in (t^n, t^{n+1})$, that
\begin{equation}
\|\frac{d^n}{dx^n} U^{\varepsilon, *}(t)\|_{L^2([a, b])} = \|\frac{d^n}{dx^n} U^{\varepsilon, *}(t)\|_{L^2([a, b])}. \nonumber
\end{equation}
and (3.17) is now obvious in view of (3.8).

**Estimation of** $R_2^\varepsilon$. From the assumptions (3.6) and (3.16) we have for $m \in \mathbb{N}$, $n = 0, 1, \ldots, N - 1$ and $t \in (t^n, t^{n+1})$,

$$
\|R_{x_1}^\varepsilon(t)\|_{L^2(a,b)} \leq \|V\|_{L^\infty(a,b)} \|T(U^\varepsilon(t)) - U^\varepsilon(t)\|_{L^2(a,b)}
$$

(3.18)

$$
\leq DB_0 \frac{\varepsilon^m}{\|x\|^{m-2}} U^\varepsilon(t) \|B_{m-2} U^\varepsilon(t)\|_{L^2(a,b)}
$$

and

$$
\|R_{x_2}^\varepsilon(t)\|_{L^2(a,b)} \leq D \frac{\varepsilon^m}{\|x\|^{m-2}} (V(x) U^\varepsilon(t)) \|B_{m-2} U^\varepsilon(t)\|_{L^2(a,b)}
$$

(3.19)

Using Leibniz’s rule we get

$$
\frac{\partial^m}{\partial x^m} U^\varepsilon(x, t) = e^{-iV(x) t/\varepsilon} U^\varepsilon(t) \frac{\partial^m}{\partial x^m} \frac{\partial^j}{\partial x^j} e^{-iV(x) t/\varepsilon} \frac{\partial^{m-j}}{\partial x^{m-j}} U^\varepsilon(t).
$$

Therefore, by assumption (3.6) and relation (3.17), we conclude that

$$
\|\frac{\partial^m}{\partial x^m} U^\varepsilon(t)\|_{L^2(a,b)} \leq \sum_{j=0}^{m} \left( \sum_{j=0}^{m-j} E_j(t) C_{m-j}, \right)
$$

where $E_0(t) = 1$ and for $j = 1, \ldots, m$, the quantities $E_j(t)$ depend only on $B_1, \ldots, B_j$ and $t - t^n$. Using the above relation in (3.18) we have

$$
\|R_{x_1}^\varepsilon(t)\|_{L^2(a,b)} \leq DB_0 \frac{\varepsilon^m (b-a)^m}{\|x\|^{m-2}} \sum_{j=0}^{m} \left( \sum_{j=0}^{m-j} E_j(t) C_{m-j}, \right)
$$

from where we conclude that for $t \in (t^n, t^{n+1})$ it holds

(3.20)

$$
\|R_{x_1}^\varepsilon(t)\|_{L^2(a,b)} \leq S^1_{m}(t) \left( \frac{h}{\varepsilon (b-a)} \right)^m,
$$

where the terms $S^1_{m}(t)$ remain bounded while $k$ and $\varepsilon$ tend to zero.

Using again Leibniz’s rule, we obtain

$$
\frac{\partial^m}{\partial x^m} (V(x) U^\varepsilon(t)) = \sum_{j=0}^{m} \left( \sum_{j=0}^{m-j} \frac{d_j}{d x^j} V(x) \frac{\partial^{m-j}}{\partial x^{m-j}} U^\varepsilon(t), \right)
$$

From assumption (3.6) and (3.17) we have

$$
\|\frac{\partial^m}{\partial x^m} (V(x) U^\varepsilon(t))\|_{L^2(a,b)} \leq \sum_{j=0}^{m} \left( \sum_{j=0}^{m-j} \frac{1}{\varepsilon^{m-j}} B_j \sum_{j=0}^{m-j} \left( \sum_{j=0}^{m-j} C_{m-j-\ell}, \right) E_{\ell}(t) C_{m-j-\ell}, \right)
$$

where $E_0(t), E_1(t), \ldots, E_m(t)$ are as before. Thus, for $t \in (t^n, t^{n+1})$ and $m \in \mathbb{N}$, we obtain the estimate

(3.21)

$$
\|R_{x^2}^\varepsilon(t)\|_{L^2(a,b)} \leq S^2_{m}(t) \left( \frac{h}{\varepsilon (b-a)} \right)^m,
$$

where again the terms $S^2_{m}(t)$ remain bounded while $k$ and $\varepsilon$ tend to zero.

From the definition of $R_{x^2}^\varepsilon$ and (3.16) we obtain for $t \in (t^n, t^{n+1})$, $n = 0, 1, \ldots, N - 1$ and $m \in \mathbb{N}$,

$$
\|R_{x^2}^\varepsilon(t)\|_{L^2(a,b)} \leq \varepsilon^2 \frac{\partial^2}{\partial x^2} (U^\varepsilon(t) - T(U^\varepsilon(t))) \|B_{m-2} U^\varepsilon(t)\|_{L^2(a,b)}
$$

$$
\leq \frac{\varepsilon^2}{2} D \frac{\varepsilon^2}{\|x\|^{m-2}} U^\varepsilon(t) \|B_{m-2} U^\varepsilon(t)\|_{L^2(a,b)} (b-a)^m.
$$
Proceeding as in the estimation of $R^\varepsilon_{s_1}$, we obtain
\[
\left\| \frac{\partial^{m+2}}{\partial x^{m+2}} U^\varepsilon(t) \right\|_{L^2(a,b)} \leq \frac{1}{\varepsilon^{m+2}} \sum_{j=0}^{m+2} \binom{m+2}{j} E_j(t) C_{m+2-j},
\]
so that
\[
\left\| R^\varepsilon_{s_2}(t) \right\|_{L^2(a,b)} \leq \frac{D \varepsilon^2}{2} \left( \frac{h}{b-a} \right)^m \sum_{j=0}^{m+2} \binom{m+2}{j} E_j(t) C_{m+2-j}.
\]
From the above relation we conclude, for $m \in \mathbb{N}$ and $t \in (t^n, t^{n+1})$, the estimate
\[
(3.22) \quad \left\| R^\varepsilon_{s_3}(t) \right\|_{L^2(a,b)} \leq S^4_m(t) \left( \frac{h}{\varepsilon(b-a)} \right)^m,
\]
with $S^4_m(t)$ remaining bounded as $k$ and $\varepsilon$ tend to zero.

Finally, using the definition of $R^\varepsilon_{s_4}$ we have, for $m \in \mathbb{N}$ and $t \in (t^n, t^{n+1}), n = 0, \ldots, N-1,$
\[
\left\| R^\varepsilon_{s_4}(t) \right\|_{L^2(a,b)} \leq D \frac{\varepsilon^2}{2} \left( \frac{h}{b-a} \right)^m \sum_{j=0}^{m+2} \binom{m+2}{j} E_j(t) C_{m+2-j},
\]
and therefore we obtain the estimate
\[
(3.23) \quad \left\| R^\varepsilon_{s_4}(t) \right\|_{L^2(a,b)} \leq S^4_m(t) \left( \frac{h}{\varepsilon(b-a)} \right)^m,
\]
where the terms $S^4_m(t)$ remain bounded as $k$ and $\varepsilon$ tend to zero.

**Estimation of $R^\varepsilon_{t_m}$.** Recall that for $x \in [a, b]$ and $t \in (t^n, t^{n+1}), n = 0, 1, \ldots, N-1,$ we have
\[
R^\varepsilon_{t_m}(x, t) = \varepsilon^2 \left( e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{xx}(x, t) - e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x,x}(x, t) \right).
\]
A simple calculation reveals that
\[
e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{xx}(x, t) - e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x,x}(x, t) = \frac{i}{\varepsilon} \left( t - t^n \right) V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t) + \frac{(t-t^n)^2}{\varepsilon^2} \left( V''(x) \right) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t) + i \varepsilon \left( t - t^n \right) V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t).
\]
We write $R^\varepsilon_{t_m}(x, t) = R^\varepsilon_{t_{m_1}}(x, t) + R^\varepsilon_{t_{m_2}}(x, t) + R^\varepsilon_{t_{m_2}}(x, t),$ where
\[
R^\varepsilon_{t_{m_1}}(x, t) = -\frac{\varepsilon}{2} \left( t - t^n \right) V''(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t),
\]
\[
R^\varepsilon_{t_{m_2}}(x, t) = \frac{1}{2} \left( t - t^n \right)^2 \left( V''(x) \right) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t),
\]
\[
R^\varepsilon_{t_{m_3}}(x, t) = -\varepsilon \left( t - t^n \right) V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t).
\]
Relations (3.16), (3.17) and assumption (3.6) give
\[
\left\| T \left( V''(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t) \right) \right\|_{L^2(a,b)} \leq
\]
\[
D \left( \frac{h}{b-a} \right)^m \left\| \frac{\partial^m}{\partial x^m} (V''(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t)) \right\|_{L^2(a,b)} + B_2 C_0,
\]
and
\[
\left\| T \left( V''(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t) \right) \right\|_{L^2(a,b)} \leq
\]
\[
D \left( \frac{h}{b-a} \right)^m \left\| \frac{\partial^m}{\partial x^m} (V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t)) \right\|_{L^2(a,b)} + B_2 C_0.
\]
and
\[
\left\| T \left( V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t) \right) \right\|_{L^2(a,b)} \leq
\]
\[
D \left( \frac{h}{b-a} \right)^m \left\| \frac{\partial^m}{\partial x^m} (V'(x) e^{-iV(x)\frac{t-t^n}{\varepsilon}} U^\varepsilon_{x}(x, t)) \right\|_{L^2(a,b)} + \frac{1}{\varepsilon} B_1 C_1.
\]
Proceeding as in the estimation of the term $R^c$, we obtain, for $m \in \mathbb{N}$ and $t \in (t^n, t^{n+1})$, $n = 0, 1, \ldots, N - 1$, the estimates
\begin{equation}
\|R^c_{t^m_1}(t)\|_{L^2(a, b)} \leq T^1_m(t)\varepsilon(t - t^n),
\end{equation}
where the quantities $T^1_m(t)$, $T^2_m(t)$ and $T^3_m(t)$ remain, under the assumption (3.9), bounded as $k, h$ and $\varepsilon$ tend to zero.

We collect our results so far in the following lemma.

**Lemma 3.1.** Under assumptions (3.5) and (3.6) we have, for $x \in [a, b]$ and $t \in (t^n, t^{n+1})$, $n = 0, 1, \ldots, N - 1$, that for all positive integers $m$,
\begin{align*}
\|R^c_{t^m_1}(t)\|_{L^2(a, b)} &\leq S^1_m(t)\left(\frac{\varepsilon}{b - a}\right)^m, \quad i = 1, \ldots, 4, \\
\|R^c_{t^m_1}(t)\|_{L^2(a, b)} &\leq S^2_m(t)\left(\frac{\varepsilon}{b - a}\right)^m, \quad j = 1, 2, 3,
\end{align*}
where $\alpha(1) = 1$, $\alpha(2) = 3 = 0$ and $\beta(1) = 3 = 1$, $\beta(2) = 2$. Furthermore, assuming the mesh condition (3.9), the quantities $S^i_m$, $i = 1, \ldots, 4$, and $T^j_m$, $j = 1, 2, 3$, remain bounded as $k, h$ and $\varepsilon$ tend to zero. In particular, for all positive integers $m$, the following estimate for the residual holds:
\begin{equation}
\sup_{0 \leq t \leq T} \|R^c(t)\|_{L^2(a, b)} = O\left(\frac{h^m}{(\varepsilon (b - a))^m}\right) + O(k).
\end{equation}

In view of Theorem 3.1 and Lemma 3.1, we immediately conclude the following

**Corollary 3.1.** Let $u^\varepsilon$ be the solution of problem (2.1)–(2.3) and $U^\varepsilon_I$ the continuous Lie splitting approximation (2.16). Then, under assumptions (3.5), (3.6) and the mesh condition (3.9) we have
\begin{equation}
\max_{0 \leq t \leq T} \|u^\varepsilon(t) - U^\varepsilon_I(t)\|_{L^2(a, b)} = O\left(\frac{\varepsilon^m + 1}{(b - a)^m}\right) + O\left(\frac{h}{\varepsilon}\right).
\end{equation}

**Remark 3.3.** If $V(x) \equiv V$ is a constant electrostatic potential then $R^c(t) \equiv 0$ and Theorem 3.1 implies that
\begin{equation}
\max_{0 \leq t \leq t^{n+1}} \|u^\varepsilon(t) - U^\varepsilon_I(t)\|_{L^2(a, b)} \leq \|u^\varepsilon_0 - T^1 u^\varepsilon_0\|_{L^2(a, b)} = O\left(\frac{h^m}{(\varepsilon (b - a))^m}\right),
\end{equation}
and the time steps $k_1, \ldots, k_{N-1}$ can be chosen independently of $\varepsilon$.

## 4. Proof of Proposition 3.1

In this section we will give the basic ideas that lead us to the proof of Proposition 3.1. In the propositions and lemmas below, we shall assume that the potential $V$ is a $C^\infty$ and $(b - a)$–periodic function and that (3.5) and (3.6) hold. The proof is motivated by the work of Jahnke and Lubich [7] where a similar result for $\varepsilon = 1$ is stated without proof. An essential ingredient in our proof is a commutator estimate from [7]. We start by proving (3.8) in the case of a semidiscrete scheme where the discretization in time is achieved by the Lie splitting spectral method. The proof in this case is less technical, nevertheless it helps establishing the ideas used in the proof at the fully discrete level.

Let $e^{\frac{i}{\varepsilon} \frac{\partial^2}{\partial x^2} t_0}$ be the solution of the problem
\begin{equation}
\begin{cases}
\frac{v^\varepsilon - i \frac{\varepsilon}{2} \frac{\partial^2}{\partial x^2} v}{\partial t} = 0 & \text{in } [a, b] \times (t^n, t^{n+1}], \\
v^\varepsilon(t, t^{n+1}) = u^\varepsilon_0 & \text{in } [a, b],
\end{cases}
\end{equation}
with periodic boundary conditions, at $t = t^{n+1}$. We discretize problem (2.1)–(2.3) only in time by the Lie splitting method to obtain approximations $\{\tilde{U}^{\varepsilon, n}\}_{n=0}^{N}$ given by the numerical scheme
\begin{equation}
\begin{cases}
\tilde{U}^{\varepsilon, n+1} = e^{-iV(x) k_n} e^{\frac{i}{\varepsilon} \frac{\partial^2}{\partial x^2} t_n} \tilde{U}^{\varepsilon, n}, & n = 0, 1, \ldots, N - 1, \\
\tilde{U}^{\varepsilon, 0} = u^\varepsilon_0,
\end{cases}
\end{equation}
Proposition 4.1. Let \( \{\hat{U}^\varepsilon_n\}_{n=0}^N \) be the approximations obtained by (4.1). Then for \( m \in \mathbb{N}_0 \), there exist positive constants \( C_m \) which remain bounded while \( \varepsilon \) tends to zero and are independent of the time step such that

\[
(4.2) \quad \max_{0 \leq n \leq N} \| \frac{d^n}{dx^n} \hat{U}^\varepsilon_n \|_{L^2(a,b)} \leq \frac{\tilde{C}_m}{\varepsilon^m}.
\]

Proof. First of all it is easy to verify that

\[
||\hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} = ||\hat{U}^\varepsilon_n||_{L^2(a,b)}, \quad n = 0, 1, \ldots, N - 1,
\]
or

\[
||\hat{U}^\varepsilon_n||_{L^2(a,b)} = ||v_0||_{L^2(a,b)}, \quad n = 0, 1, \ldots, N.
\]

In view of hypothesis (3.5), we arrive at

\[
(4.3) \quad \max_{0 \leq n \leq N} ||\hat{U}^\varepsilon_n||_{L^2(a,b)} \leq A_0,
\]

and thus (4.2) is valid for \( m = 0 \) with \( \tilde{C}_0 = A_0 \).

On the other hand, using the numerical scheme (4.1), we obtain

\[
\frac{d}{dx} \hat{U}^\varepsilon_{n+1} = -\frac{k_n}{\varepsilon} V'(x)e^{-iV(x)} \frac{\partial^2}{\partial x^2} \hat{U}^\varepsilon_n + e^{-iV(x)} \frac{\partial}{\partial x} \hat{U}^\varepsilon_n.
\]

The operators \( \frac{d}{dx} \) and \( e^{i\frac{\partial}{\partial x}} \frac{\partial^2}{\partial x^2} \) commute on the space of periodic smooth functions, so

\[
\frac{d}{dx} \hat{U}^\varepsilon_{n+1} = -\frac{k_n}{\varepsilon} V'(x)e^{-iV(x)} \frac{\partial^2}{\partial x^2} \hat{U}^\varepsilon_n + e^{-iV(x)} \frac{\partial}{\partial x} \hat{U}^\varepsilon_n,
\]

and thus

\[
||\frac{d}{dx} \hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} \leq \frac{k_n}{\varepsilon} ||V'||_{L^\infty(a,b)} ||\hat{U}^\varepsilon_n||_{L^2(a,b)} + ||\frac{d}{dx} \hat{U}^\varepsilon_n||_{L^2(a,b)},
\]

or by virtue of (4.3),

\[
||\frac{d}{dx} \hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} \leq \frac{k_n}{\varepsilon} ||V'||_{L^\infty(a,b)} A_0 + ||\frac{d}{dx} \hat{U}^\varepsilon_n||_{L^2(a,b)}, \quad n = 0, 1, \ldots, N - 1.
\]

Using now induction on \( n \) and the fact that \( \frac{d}{dx} \hat{U}^\varepsilon_0 = \frac{d}{dx} u_0 \), we obtain

\[
(4.4) \quad ||\frac{d}{dx} \hat{U}^\varepsilon_n||_{L^2(a,b)} \leq \frac{1}{\varepsilon} (k_0 + \cdots + k_{n-1}) ||V'||_{L^\infty(a,b)} A_0 + ||\frac{d}{dx} u_0||_{L^2(a,b)},
\]

hence in light of assumptions (3.5) and (3.6),

\[
(4.5) \quad \max_{0 \leq n \leq N} ||\frac{d}{dx} \hat{U}^\varepsilon_n||_{L^2(a,b)} \leq \frac{1}{\varepsilon} (TB_1 A_0 + A_1),
\]

and therefore (4.2) holds for \( m = 1 \) as well, with \( \tilde{C}_1 = TB_1 A_0 + A_1 \).

Similar arguments as before, and Leibniz’s rule yield that

\[
||\frac{d^2}{dx^2} \hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} \leq k_n \frac{B_2^2 A_0}{\varepsilon^2} + 2k_n \frac{B_1}{\varepsilon} ||\frac{d}{dx} \hat{U}^\varepsilon_n||_{L^2(a,b)} + k_n \frac{B_2 A_0}{\varepsilon} + ||\frac{d^2}{dx^2} \hat{U}^\varepsilon_n||_{L^2(a,b)},
\]

and thus in view of (4.4),

\[
||\frac{d^2}{dx^2} \hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} \leq k_n \frac{B_2^2 A_0}{\varepsilon^2} + 2k_n \frac{B_1}{\varepsilon} \left( (k_0 + \cdots + k_{n-1}) B_1 A_0 + A_1 \right) + ||\frac{d^2}{dx^2} \hat{U}^\varepsilon_n||_{L^2(a,b)}, \quad n = 0, 1, \ldots, N - 1.
\]

Using induction on \( n \), and combining (3.5) and the fact that \( \frac{d^2}{dx^2} \hat{U}^\varepsilon_n = \frac{d^2}{dx^2} u_0 \), we get

\[
||\frac{d^2}{dx^2} \hat{U}^\varepsilon_{n+1}||_{L^2(a,b)} \leq (k_0 + \cdots + k_n) \frac{B_2 A_0}{\varepsilon^2} + 2(k_0 + \cdots + k_n) \frac{B_1}{\varepsilon} A_2 + \frac{A_2}{\varepsilon^2}, \quad n = 0, 1, \ldots, N - 1,
\]
Therefore (4.2) is also valid for \( m = 2 \) with 
\[
\tilde{C}_2 = \varepsilon TB_2 A_0 + 2TB_1 A_1 + T^2 B_1^2 A_0 + A_2.
\]

It is now obvious that by double induction on \( n \) and \( m \), we can prove (4.2) with \( \tilde{C}_m \) depending only \( A_0, A_1, \ldots, A_m, B_1, \ldots, B_m \) and \( T, \ldots, T^m \), and remaining bounded while \( \varepsilon \) tends to zero. \( \square \)

In the sequel, we will use the formalism of Section 3 in \cite{7}. Let \( \mathcal{F}_M = [e^{-i\mu_\ell(x_\ell-a)}]_{\ell=0}^{2M} \) be the discrete Fourier transform and \( \mathcal{F}_M^{-1} = \frac{1}{M} \mathcal{F}^* \) be the inverse discrete Fourier transform. For \( n = 0, 1, \ldots, N \), we define the vector \( \hat{U}^{\varepsilon,n} \in \mathbb{C}^M \) as 
\[
\hat{U}^{\varepsilon,n} \ := \ [\hat{U}^{\varepsilon,n}_\ell]_{\ell=0}^{2M},
\]
where \( \hat{U}^{\varepsilon,n}_\ell \) are given by (2.9). Then, it can easily be verified (see \cite[Section 3]{7}) that \( \hat{U}^{\varepsilon,n} \), \( n = 0, 1, \ldots, N \), may also be computed via the following numerical scheme
\[
\begin{aligned}
\hat{U}^{\varepsilon,n+1} &= e^{-\frac{i}{2M}W \hat{U}^{\varepsilon,n} D^2} \hat{U}^{\varepsilon,n}, \quad n = 0, 1, \ldots, N - 1, \\
\hat{U}^{\varepsilon,0} &= \mathcal{F}_M[v_0^\varepsilon(x_\ell)]_{\ell=0}^{2M},
\end{aligned}
\]
where the matrices \( W \) and \( D \) are defined as
\[
W := \mathcal{F}_M \text{diag}[V(x_\ell)] \mathcal{F}_M^{-1}
\]
and
\[
D := \text{diag}[i\mu_\ell],
\]
respectively.

For \( v = [v_\ell]_{\ell=0}^{2M} \in \mathbb{C}^M \), we define
\[
||v||_2^2 := (b-a) \sum_{\ell=-M}^{M-1} |v_\ell|^2.
\]

**Lemma 4.1.** For every \( m \in \mathbb{N}_0 \) and \( n = 0, 1, \ldots, N \),
\[
||\frac{d^m}{dx^m} U^{\varepsilon,n}_I||_{L^2(a,b)} = ||\mathcal{D}^m \hat{U}^{\varepsilon,n}||_{L^2},
\]
where \( U^{\varepsilon,n}_I \), \( n = 0, 1, \ldots, N \), are given by (2.10).

**Proof.** First of all notice that
\[
||\frac{d^m}{dx^m} U^{\varepsilon,n}_I||_{L^2(a,b)}^2 = (b-a) \sum_{\ell=-M}^{M-1} (i\mu_\ell)^{2m} |\hat{U}^{\varepsilon,n}_\ell|^2.
\]

Here we have used that
\[
\langle e^{i\mu_\ell(-a)}, e^{i\mu_m(-a)} \rangle_{L^2(a,b)} = \begin{cases} b-a & \text{if } \ell = m \\ 0 & \text{if } \ell \neq m, \end{cases}
\]
where \( \langle \cdot, \cdot \rangle_{L^2(a,b)} \) denotes the inner product in \( L^2(a,b) \). On the other hand, it is easy to see that
\[
||\mathcal{D}^m \hat{U}^{\varepsilon,n}||_{L^2}^2 = (b-a) \sum_{\ell=-M}^{M-1} (i\mu_\ell)^{2m} |\hat{U}^{\varepsilon,n}_\ell|^2,
\]
from which (4.9) follows. \( \square \)

**Lemma 4.2.** For every \( v \in \mathbb{C}^M \),
\[
\text{Re}\{iWv, v\}_{L^2(a,b)} = 0,
\]
where \( W \) is the matrix in (4.7).
Proof. To show (4.10), it is enough to show that \((Wv, v)_{L^2(a,b)}\) is a real number for every \(v \in \mathbb{C}^M\). Indeed,
\[
(Wv, v)_{L^2(a,b)} = (\mathcal{F}_M \text{diag}[V(x_t)] \mathcal{F}_M^{-1} v, v)_{L^2(a,b)} = (\text{diag}[V(x_t)] \mathcal{F}_M^* v, \mathcal{F}_M v)_{L^2(a,b)},
\]
and since \(\text{diag}[V(x_t)]\) is diagonal and real, we have that \((\text{diag}[V(x_t)] \mathcal{F}_M^* v, \mathcal{F}_M v)_{L^2(a,b)} \in \mathbb{R}\) or \((Wv, v)_{L^2(a,b)} \in \mathbb{R}\), and therefore the proof is complete. \(\Box\)

The following lemma is a simple variation on commutator estimates given by Jahnke and Lubich, [7, Lemma 3.1].

**Lemma 4.3.** For every \(m \in \mathbb{N}\), there exists a positive constant \(c_m\) independent of the space (and time) step (and of \(\varepsilon\)) such that for every \(v \in \mathbb{C}^M\),
\[
\|(D^m W - WD^m) v\|_{L^2(a,b)} \leq c_m \|D^{m-1} v\|_{L^2(a,b)}.
\]

Having in hand the three lemmas above, we can now prove Proposition 3.1. The proof is detailed, since we are interested in keeping track on the dependence of various constants on \(\varepsilon\).

**Proof of Proposition 3.1.** First of all, by the numerical scheme (4.6), it is easily seen that (see also [1, Lemma 3.1])
\[
||\hat{U}_{\varepsilon,n+1}||_2 = ||\hat{U}_{\varepsilon,n}||_2, \quad n = 0, 1, \ldots, N - 1,
\]
or
\[
||\hat{U}_{\varepsilon,n}||_2 = ||\hat{U}_{\varepsilon,0}||_2, \quad n = 0, 1, \ldots, N.
\]
Hence, in view of (4.9),
\[
||U_{\varepsilon,n}||_{L^2(a,b)} = ||U_{\varepsilon,0}||_{L^2(a,b)}, \quad n = 0, 1, \ldots, N.
\]
Since \(||U_{\varepsilon,0}||_{L^2(a,b)} = ||Tu_0||_{L^2(a,b)}\), we obtain
\[
\max_{0 \leq n \leq N} ||U_{\varepsilon,n}||_{L^2(a,b)} = ||Tu_0||_{L^2(a,b)}.
\]
Using now assumption (3.5) and (3.16) we conclude that
\[
\max_{0 \leq n \leq N} ||U_{\varepsilon,n}||_{L^2(a,b)} \leq ||Tu_0 - u_0||_{L^2(a,b)} + ||u_0||_{L^2(a,b)} \leq (D + 1)A_0,
\]
where \(D\) and \(A_0\) are the constants appearing in (3.16) and assumption (3.5), respectively. Therefore, (3.8) holds for \(m = 0\) with \(C_0 = (D + 1)A_0\).

For \(n = 0, 1, \ldots, N - 1\), let us consider the function
\[
\hat{U}_{\varepsilon}(t) := e^{-i\frac{\varepsilon}{\tau}W} e^{i\frac{\varepsilon}{\tau}(t-t^n)D^2} \hat{U}_{\varepsilon,n}, \quad t \in (t^n, t^{n+1}].
\]
Then, obviously \(\hat{U}_{\varepsilon}(t^{n+1}) = \hat{U}_{\varepsilon,n}\) and \(\hat{U}_{\varepsilon}(t^{n+1}) = \hat{U}_{\varepsilon,n+1}\), in light of (4.6). Also, for \(t \in (t^n, t^{n+1}]\),
\[
D\hat{U}_{\varepsilon}(t) = D e^{-i\frac{\varepsilon}{\tau}W} e^{i\frac{\varepsilon}{\tau}(t-t^n)D^2} \hat{U}_{\varepsilon,n} + (D e^{-i\frac{\varepsilon}{\tau}W} e^{i\frac{\varepsilon}{\tau}(t-t^n)D^2} \hat{U}_{\varepsilon,n}) (D e^{-i\frac{\varepsilon}{\tau}W} e^{i\frac{\varepsilon}{\tau}(t-t^n)D^2} \hat{U}_{\varepsilon,n})
\]
(4.13)
Let \(v_1(t) := e^{-i\frac{\varepsilon}{\tau}W} v_0\), \(t \in (t^n, t^{n+1}].\) Then by definition, \(v_1\) satisfies the problem
\[
\left\{ \begin{array}{l}
v_1(t) = -i W v_1, \quad t \in (t^n, t^{n+1}], \\
v_1(t^{n+1}) = v_0.
\end{array} \right.
\]
Therefore, \(Dv_1\) satisfies the problem
\[
\left\{ \begin{array}{l}
(Dv_1)(t) = -i W v_1, \quad t \in (t^n, t^{n+1}], \\
(Dv_1)(t^{n+1}) = Dv_0.
\end{array} \right.
\]
Similarly, let \(v_2(t) := e^{-i\frac{\varepsilon}{\tau}W} (Dv_0)\), \(t \in (t^n, t^{n+1}].\) Again, by definition, \(v_2\) satisfies the problem
\[
\left\{ \begin{array}{l}
v_2(t) = -i W v_2, \quad t \in (t^n, t^{n+1}], \\
v_2(t^{n+1}) = Dv_0.
\end{array} \right.
\]
So,
\[(Dv_1^\varepsilon - v_2^\varepsilon)_t = -\frac{i}{\varepsilon}DWv_1^\varepsilon + \frac{i}{\varepsilon}Wv_2^\varepsilon = -\frac{i}{\varepsilon}DWv_1^\varepsilon + \frac{i}{\varepsilon}WDv_1^\varepsilon - \frac{i}{\varepsilon}W(Dv_1^\varepsilon - v_2^\varepsilon).\]

In other words, the difference \(Dv_1^\varepsilon - v_2^\varepsilon\) satisfies the problem
\[
\begin{aligned}
(Dv_1^\varepsilon - v_2^\varepsilon)_t &= \frac{i}{\varepsilon}W(Dv_1^\varepsilon - v_2^\varepsilon) + \frac{i}{\varepsilon}(WD - DW)v_1^\varepsilon, \quad t \in (t^n, t^{n+1}], \\
(Dv_1^\varepsilon - v_2^\varepsilon)(t^n) &= 0.
\end{aligned}
\]

Taking the \(L^2\)-inner product with \(Dv_1^\varepsilon - v_2^\varepsilon\) and then real parts we establish, in light of (4.10) and of (4.11), that
\[
\begin{aligned}
d &\frac{d}{dt}||\langle Dv_1^\varepsilon - v_2^\varepsilon \rangle(t)||_2 \leq \frac{1}{\varepsilon}c_1 \int_{t^{n-1}}^{t^n} ||v_1^\varepsilon(t)||_2 dt,
\end{aligned}
\]
where \(c_1\) is the constant appearing in (4.11) with \(m = 1\). Recall now that \(v_1^\varepsilon(t) = e^{-\frac{\varepsilon}{2}w(t)} Wv_0\) and \(v_2^\varepsilon(t) = e^{-\frac{\varepsilon}{2}w(t)} WDv_0\), and set \(v_0 = e^{i\varepsilon k_n D^2 \hat{U}^\varepsilon, n}\). Then, for \(t \in (t^n, t^{n+1}]\), we derive in view of (4.12) that
\[
||v_1^\varepsilon(t)||_2 = ||e^{-\frac{\varepsilon}{2}w(t)} WU_0^{\hat{U}^\varepsilon, n}||_2 = ||U_0^{\hat{U}^\varepsilon, 0}||_2 = ||\hat{U}^{\varepsilon, 0}||_2.
\]

Therefore we have in view of (4.14) (with \(t = t^{n+1}\)),
\[
||\langle D(e^{-i\varepsilon w/2} - e^{-i\varepsilon w/2} D)e^{i\varepsilon k_n D^2 \hat{U}^\varepsilon, n} \rangle||_2 \leq \frac{1}{\varepsilon}c_1 k_n ||\hat{U}^{\varepsilon, 0}||_2.
\]

Combining now (4.13) (with \(t = t^{n+1}\)) and (4.15) we obtain
\[
||\hat{U}^{\varepsilon, n+1}||_2 \leq ||\hat{U}^{\varepsilon, n}||_2 + \frac{1}{\varepsilon}c_1 k_n ||\hat{U}^{\varepsilon, 0}||_2, \quad n = 0, 1, \ldots, N - 1,
\]
and thus by induction on \(n\),
\[
||\hat{U}^{\varepsilon, n}||_2 \leq \frac{1}{\varepsilon}c_1 T ||\hat{U}^{\varepsilon, 0}||_2 + ||\hat{D}^{\varepsilon, 0}||_2.
\]

(4.9) and (4.16) ensure that
\[
||\frac{d}{dx}U^{\varepsilon, n}_{f}\||_{L^2(a,b)} \leq \frac{1}{\varepsilon}c_1 T ||U^{\varepsilon, 0}_{f}\||_{L^2(a,b)} + ||\frac{d}{dx}U^{\varepsilon, 0}_{f}\||_{L^2(a,b)}.
\]

Since \(U^{\varepsilon, 0}_{f} = Tu_0\) we obtain, in view of (3.5) and (3.16), that
\[
\max_{0 \leq n \leq N} ||\frac{d}{dx}U^{\varepsilon, n}_{f}\||_{L^2(a,b)} \leq \frac{1}{\varepsilon}(D + 1)(c_1 TA_0 + A_1).
\]

Notice that (4.17) is of the same form of (4.5) in the semidiscrete scheme. Therefore (3.8) holds for \(m = 1\) as well with \(C_1 = (D + 1)(c_1 TA_0 + A_1)\).

Using now similar arguments as above we can prove (in the spirit of the proof of Proposition 4.1 for \(m = 2\) (3.8) with \(C_2\) depending on \(D, A_0, A_1, A_2, c_1, c_2, T\) and \(T^2\) and remaining bounded while \(\varepsilon\) tends to zero.

More generally, we can prove, by double induction on \(n\) and \(m\), (3.8) with \(C_m\) depending on \(D, A_0, A_1, \ldots, A_m, c_1, \ldots, c_m, T, \ldots, T^m\) and remaining bounded while \(\varepsilon\) tends to zero.

5. A posteriori error analysis of the Strang splitting spectral method

Another well-known time-splitting method for problem (2.1)–(2.3) is Strang’s method, see, e.g., [7], [5] and [2]. In [1], where we refer for the derivation and a priori error analysis, it was shown...
that Strang’s method is of second order in $k$ for any fixed $\varepsilon > 0$. Strang’s splitting spectral method computes approximations $U^{\varepsilon,n}_{j}$ to $u^{\varepsilon}(x_{j}, t^{n})$ by means of

\begin{align}
U^{\varepsilon,0}_{j} &= u_{0}^{\varepsilon}(x_{j}), \quad j = 0, 1, \ldots, M - 1, \\
U^{\varepsilon,*}_{j} &= e^{-iV(x_{j})\frac{\Delta t}{M}} U^{\varepsilon,n}_{j}, \quad j = 0, 1, \ldots, M - 1, \\
U^{\varepsilon,**}_{j} &= \frac{1}{M} \sum_{\ell = -M/2}^{M/2-1} e^{-i\frac{\ell t}{M}\mu^{2}} \hat{U}^{\varepsilon,*}_{\ell} e^{i\mu(x_{j}-a)}, \quad j = 0, 1, \ldots, M - 1, \\
U^{\varepsilon,n+1}_{j} &= e^{-iV(x_{j})\frac{\Delta t}{M}} U^{\varepsilon,**}_{j}, \quad j = 0, 1, \ldots, M - 1,
\end{align}

where $\hat{U}^{\varepsilon,*}_{\ell}$ are defined by

\begin{equation}
\mu_{\ell} = \frac{2\pi\ell}{b-a}, \quad \hat{U}^{\varepsilon,*}_{\ell} = \sum_{j=0}^{M-1} U^{\varepsilon,*}_{j} e^{-i\mu_{\ell}(x_{j}-a)}, \quad \ell = -M/2, \ldots, M/2 - 1.
\end{equation}

For $n = 0, 1, \ldots, N$ and $x \in [a, b]$, the approximations of the exact solution $u^{\varepsilon}$ at the nodes $t^{n}$ are given by

\begin{equation}
U^{\varepsilon,n}_{j}(x) = \frac{1}{M} \sum_{\ell = -M/2}^{M/2-1} \hat{U}^{\varepsilon,n}_{\ell} e^{i\mu_{\ell}(x-a)},
\end{equation}

with $\hat{U}^{\varepsilon,n}_{\ell}, \ell = -M/2, \ldots, M/2 - 1$, as in (2.9).

Proceeding as in the case of the Lie time-splitting spectral approximation, we introduce the continuous Strang splitting approximation $U^{\varepsilon}_{I} : [a, b] \times [0, T] \to \mathbb{C}$, a continuous in time and space function that coincides with the approximations $U^{\varepsilon,n}_{I}$ at the nodes $t^{n}$, $n = 0, 1, \ldots, N$. To this end, we first let

\begin{equation}
U^{\varepsilon}(x, 0) = u_{0}^{\varepsilon}(x), \quad x \in [a, b].
\end{equation}

Then, for $x \in [a, b]$ and $t \in (t^{n}, t^{n+1}]$, $n = 0, 1, \ldots, N - 1$, we define

\begin{align}
U^{\varepsilon,*}_{I}(x, t) &= e^{-iV(x)\frac{t-t^{n}}{M}} U^{\varepsilon}(x, t^{n}), \\
U^{\varepsilon,**}_{I}(x, t) &= \frac{1}{M} \sum_{\ell = -M/2}^{M/2-1} e^{-i\frac{\ell t}{M}\mu^{2}} \hat{U}^{\varepsilon,*}_{\ell}(t) e^{i\mu_{\ell}(x-a)}, \\
U^{\varepsilon}_{I}(x, t) &= e^{-iV(x)\frac{t-t^{n}}{M}} U^{\varepsilon,**}_{I}(x, t),
\end{align}

where

\begin{equation}
\hat{U}^{\varepsilon,*}_{\ell}(t) = \sum_{j=0}^{M-1} U^{\varepsilon,*}_{j}(x_{j}, t)e^{-i\mu_{\ell}(x_{j}-a)}, \quad \ell = -M/2, \ldots, M/2 - 1.
\end{equation}

The continuous Strang splitting approximation $U^{\varepsilon}_{I}$ of the exact solution $u^{\varepsilon}$ is defined as

\begin{equation}
U^{\varepsilon}_{I}(x, t) = \frac{1}{M} \sum_{\ell = -M/2}^{M/2-1} \hat{U}^{\varepsilon}_{\ell}(t) e^{i\mu_{\ell}(x-a)},
\end{equation}

with $\hat{U}^{\varepsilon}_{\ell} : (t^{n}, t^{n+1}] \to \mathbb{C}$, $\ell = -M/2, \ldots, M/2 - 1$, denoting the time-continuous Fourier coefficients of $U^{\varepsilon}$, see (2.15).

For the purpose of the a posteriori error analysis we introduce yet another trigonometric interpolation operator: For $n = 0, 1, \ldots, N - 1$ and each fixed $\varepsilon$, the operators $T^{n,*} : C([a, b] \times (t^{n}, t^{n+1}]) \to C([a, b] \times (t^{n}, t^{n+1}))$ are defined by

\begin{equation}
(T^{n,*} f)(x, t) = \frac{1}{M} \sum_{\ell = -M/2}^{M/2-1} e^{-i\frac{\ell t}{M}\mu^{2}} \hat{f}_{\ell}(t) e^{i\mu_{\ell}(x-a)},
\end{equation}
with \( \hat{f}_t \) the time-continuous discrete Fourier coefficients,

\[
\hat{f}_t(t) = \sum_{j=0}^{M-1} f(x_j, t) e^{-i\omega_j(x_j-a)}.
\]

Obviously, the operators \( T^{n,\varepsilon} \) are well defined and linear. From (5.11) it follows immediately that for \( t \in (t^n, t^{n+1}) \), \( n = 0, 1, \ldots, N-1 \) and \( x \in [a, b] \) we have

\[
U^{\varepsilon,**}(x, t) = T^{n,\varepsilon}(U^{\varepsilon,*}(x, t)).
\]

A straightforward calculation reveals that, for \( n = 0, 1, \ldots, N-1 \), we have

\[
\varepsilon U_t^{\varepsilon,**} - \frac{i}{2} \varepsilon U_{xx}^{\varepsilon,**} + \frac{1}{2} T^{n,\varepsilon}(V(x)U^{\varepsilon,*}) = 0 \quad \text{in } [a, b] \times (t^n, t^{n+1}),
\]

and for \( (x, t) \in [a, b] \times [0, T] \),

\[
U_t^f(x, t) = T(e^{-iV(x)}\frac{\varepsilon}{2}) U^{\varepsilon,**}(x, t)).
\]

We introduce the residual \( R^f(x, t) = \varepsilon U_t^f(x, t) - \frac{i}{2} \varepsilon U_{xx}^f(x, t) + iV(x)U_t^f(x, t) \). Using (5.12), (5.13) and (5.14) we conclude that \( R^f(x, t) \) may be written as

\[
R^f(x, t) = R_1^f(x, t) + R_2^f(x, t),
\]

with

\[
R_1^f(x, t) = \frac{1}{2} [V(x)T(e^{-iV(x)}\frac{\varepsilon}{2}) U^{\varepsilon,**}(x, t)) - T(V(x)e^{-iV(x)}\frac{\varepsilon}{2} U^{\varepsilon,**}(x, t))],
\]

and

\[
R_2^f(x, t) = \frac{1}{2} \left( e^{-iV(x)}\frac{\varepsilon}{2} T^{n,\varepsilon}(V(x)U^{\varepsilon,*}) \right) - \left( T(e^{-iV(x)}\frac{\varepsilon}{2} T^{n,\varepsilon}(V(x)U^{\varepsilon,*})) \right).
\]

Remark 5.1. If \( V(x) \equiv V \) is a constant electrostatic potential, we can prove, as in the case of the Lie time-splitting spectral method, that the residual \( R^f \) vanishes identically in each interval \( (t^n, t^{n+1}) \), \( n = 0, 1, \ldots, N-1 \).

We begin the analysis by noting that, if we proceed as in the case of the Lie splitting spectral method, we can prove Proposition 3.1 in the case of the Strang splitting method as well. Moreover, we can prove the following, corresponding to Proposition 3.2, proposition.

Proposition 5.1. Under assumptions (3.5) and (3.6), it holds for \( m \in \mathbb{N}_0 \) that

\[
\sup_{0 \leq t \leq T} \| \frac{\partial^m}{\partial x^m} U^{\varepsilon,**}(t) \|_{L^2(a,b)} \leq C_m \varepsilon^{-m},
\]

where \( C_m, m \in \mathbb{N}_0 \), are the constants in (3.8).

Proof. Because of (5.13) we have, for \( m \in \mathbb{N}_0 \) and \( n = 0, 1, \ldots, N-1 \), that

\[
\varepsilon \left( \frac{\partial^m}{\partial x^m} U^{\varepsilon,**} \right)_t - \frac{\varepsilon^2}{2} \left( \frac{\partial^m}{\partial x^m} U^{\varepsilon,**} \right)_{xx} + \frac{1}{2} \frac{\partial^m}{\partial x^m} T^{n,\varepsilon}(V(x)U^{\varepsilon,*}) = 0, \quad \text{in } [a, b] \times (t^n, t^{n+1}).
\]

Taking in the above relation the \( L^2 \)-inner product with \( \frac{\partial^m}{\partial x^m} U^{\varepsilon,**} \) and then real parts we arrive at

\[
\frac{1}{2} \frac{d}{dt} \| \frac{\partial^m}{\partial x^m} U^{\varepsilon,**}(t) \|_{L^2(a,b)} + \text{Re} \left\{ \frac{1}{2} \left( \frac{\partial^m}{\partial x^m} T^{n,\varepsilon}(V(x)U^{\varepsilon,*}(t)), \frac{\partial^m}{\partial x^m} U^{\varepsilon,**}(t) \right)_{L^2(a,b)} \right\} = 0,
\]

where recall that \((\cdot, \cdot)_{L^2(a,b)}\) denotes the inner product in \( L^2(a,b) \). On the other hand,

\[
\text{Re} \left\{ \frac{1}{2} \left( \frac{\partial^m}{\partial x^m} T^{n,\varepsilon}(V(x)U^{\varepsilon,*}(t)), \frac{\partial^m}{\partial x^m} U^{\varepsilon,**}(t) \right)_{L^2(a,b)} \right\} = 0.
\]
This can be easily verified using the fact that
\[
\left(e^{i\mu(-a)}, e^{i\mu(-a)}\right)_{L^2(a,b)} = \begin{cases} b-a & \text{if } \ell = m, \\ 0 & \text{if } \ell \neq m, \end{cases}
\]
and (2.17). Also, from the definition of \(U^{e,*}\) we have, for \(n = 0, 1, \ldots, N - 1\),
\[
(5.21) \quad \frac{\partial^m}{\partial x^m} U^{e,*}(t^n) = \frac{d^m}{dt^m} U^{e,n}_i, \quad \text{in } [a, b].
\]

(5.18) now follows by combining (5.19)–(5.21) and (3.8).

**Remark 5.2.** If assumptions (3.5), (3.6) and (3.9) hold, then we can prove the following estimate for the residual:

\[
(5.22) \quad \sup_{0 \leq t \leq T} \|R^e(t)\|_{L^2(a,b)} = O\left(\frac{h^m}{(b-a)^m}\right) + O(k^2).
\]

We note that (5.22) can be proven by using arguments similar to those of the Lie time-splitting spectral method in Section 3. The proof in this case is lengthy and technical and since it follows the lines of the analysis in Section 3 it is not presented herein.

**Theorem 5.1.** Let \(u^e\) be the solution of problem (2.1)–(2.3) and \(U_f^e\) the continuous Strang splitting approximation (5.10). Then, for \(n = 0, 1, \ldots, N - 1\), we have

\[
(5.23) \quad \max_{0 \leq t \leq n+1} \|u^e(t) - U_f^e(t)\|_{L^2(a,b)} \leq \|u_0^e - T_0 u_0^e\|_{L^2(a,b)} + \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \frac{1}{\varepsilon} \|R^e(t)\|_{L^2(a,b)} dt.
\]

### 6. Numerical experiments

In this section we report on the outcome of some numerical experiments performed with the Lie and Strang time-splitting spectral methods applied to problem (2.1)–(2.3). In all numerical experiments reported below the initial data were of the WKB form \(u_0^e(x) = \sqrt{n_0(x)} e^{iS_0(x)/\varepsilon}\), with

\[
\sqrt{n_0(x)} = e^{-25(x-0.5)^2}, \quad S_0(x) = 1 + x, \quad x \in [-2, 2].
\]

The two time-splitting spectral methods and the corresponding a posteriori error estimators were implemented in double precision in a C program. The discrete Fourier transforms were performed by functions of the FFTW3 library documented in [4]. All calculations were run on a Pentium 4 computer under Linux using the default C compiler.

**Experiment 1.** In our first experiment we tested the a posteriori error estimates (3.1) and (5.23). We took \(V(x) = x^2/2\), which is a harmonic oscillator, \(\varepsilon = 0.0025\), \(h = 1/256\) and computed the solution of (2.1)–(2.3) up to \(T = 3.6\) for various values of the time step \(k\). The results are summarized in Table 1. We have denoted by \(E_1^e(T)\) the a posteriori error estimator of Theorem 3.1 for the Lie time-splitting spectral method and by \(E_2^e(T)\) the a posteriori error estimator of Theorem 5.1 for Strang’s method. The exact error was approximated as follows: for each method we computed a numerical solution \(u^e_{\text{ref}}\) using a very fine spatial mesh of size \(h_{\text{ref}}\) and very small time step \(k_{\text{ref}}\) and calculated

\[
(6.2) \quad \max_{0 \leq t \leq N} \|u^e_{\text{ref}}(t^n) - U_f^e(t^n)\|_{L^2(a,b)},
\]

as an approximation of the exact error. In Table 1, \(E_1^e(T)\) denotes the exact error of the Lie method and \(E_2^e(T)\) that of Strang’s method. We used \(h_{\text{ref}}^{-1} = 4096\) and \(k_{\text{ref}} = 0.00001\) in both cases. Figure 1 depicts a log-log plot of the data of Table 1. From either Table 1 or Figure 1 it is apparent that the error estimators of Theorem 3.1 and Theorem 5.1 are of the correct temporal order. Note that for this experiment \(h/\varepsilon = 1.5625\) while \(k/\varepsilon\) ranges between 0.0625 and 1.

In order to judge the quality of the error estimators presented here, we computed for each an effectivity index, defined as the ratio of the estimator to the exact error. The effectivity indices appear in Table 1 under the heading Ratio. It is seen that as \(k\) decreases, the effectivity index for the Lie time-splitting spectral method increases slowly, while that of Strang’s method is nearly constant over the entire range of values of \(k\) and has, presumably, achieved its asymptotic value.
A POSTERIORI ERROR ESTIMATES FOR THE SCHRÖDINGER EQUATION

However, strict enforcement of the mesh condition (3.9) is apparently required for both time-splitting methods.

Concerning the cost of implementing the error estimators we note that from (3.13) and (5.17) it follows that the computation of the residual for the Lie method requires five discrete Fourier transforms for each fixed \( t \), while that of Strang’s method requires seven. Since the discrete Fourier transforms are computed by \( O(M \log M) \) algorithms of the FFTW3 library the added cost to the methods is small.

\[
\begin{array}{|c|ccc|ccc|}
\hline
k & \varepsilon & \frac{E_\varepsilon^x(T)}{E_\varepsilon^y(T)} & \text{Ratio} & \varepsilon/2 & \frac{E_{\varepsilon/2}^x(T)}{E_{\varepsilon/2}^y(T)} & \text{Ratio} \\
\hline
\varepsilon & 6.9247(-2) & 3.9217(-1) & 5.66 & 1.2603(-4) & 2.3691(-4) & 1.88 \\
\varepsilon/2 & 3.4452(-2) & 1.9599(-1) & 5.69 & 3.1503(-5) & 5.9228(-5) & 1.88 \\
\varepsilon/4 & 1.7123(-2) & 9.7974(-2) & 5.71 & 7.8720(-6) & 1.4807(-5) & 1.89 \\
\varepsilon/8 & 8.3377(-3) & 4.8981(-2) & 5.87 & 1.9648(-6) & 3.7018(-6) & 1.88 \\
\varepsilon/16 & 4.0266(-3) & 2.4489(-2) & 6.08 & 4.9034(-7) & 9.2544(-7) & 1.89 \\
\hline
\end{array}
\]

Table 1. Comparison of the exact error and the a posteriori error estimator at \( T = 3.6 \) with \( \varepsilon = 0.0025 \), \( h^{-1} = 256 \) and \( V(x) = x^2/2 \).

**Experiment 2.** In our second set of experiments we chose the so-called double-well potential \( V(x) = x^2(1 - x)^2 \), cf. [13], [14], and computed the solution to (2.1)–(2.3) up to \( T = 1.0 \) with
Figure 2. Position density (left) and current density (right) as computed by the Lie method for Experiment 2, at $t = 0.85$ with $h = 1/256$, $\varepsilon = 0.01$. Inset figures show the observables near their maximal values. Solid line corresponds to $k = 0.0025$, dotted line corresponds to $k = 0.01$.

$\varepsilon = 0.01$ and $\varepsilon = 0.0025$, for various values of the step sizes $h$ and $k$. In Figure 2 we have plotted the observables (1.3) and (1.4) as computed with the Lie time-splitting method. Figure 3 shows the observables computed by the Strang time-splitting method.

We also tested the convergence of the error estimators of Theorem 3.1 and Theorem 5.1 under the meshing strategy (3.9). In Table 2 we have computed the estimator $E_1^L(T)$ of Theorem 3.1 at $t = 1.0$ with $\varepsilon = 0.01$. In Table 3 we have computed the estimator $E_2^S(T)$ of Theorem 5.1 at $t = 1.0$ with $\varepsilon = 0.01$. Under the heading Rate in Table 2 and Table 3 we have computed the convergence rates of the two estimators. The convergence rate corresponding to two different runs with temporal sizes $k_1$ and $k_2$ and corresponding estimator values $E_1$ and $E_2$ is defined to be $\log(E_1/E_2)/\log(k_1/k_2)$, as usual. The estimators and their convergence rates for the case $\varepsilon = 0.0025$ appear in Table 4 and Table 5. From these tables it is evident that the numerically

Figure 3. Position density (left) and current density (right) as computed by the Strang method for Experiment 2, at $t = 0.85$ with $h = 1/256$, $\varepsilon = 0.01$. Inset figures show the observables near their maximal values. Solid line corresponds to $k = 0.0025$, dotted line corresponds to $k = 0.01$. Observables agree to line thickness.
observed temporal convergence rate for the $L^\infty(L^2)$ error is one for the Lie method and two for Strang’s method.

Acknowledgments

The authors would like to thank Christian Lubich for a constructive communication and his suggestions concerning [7], and George Makrakis for useful discussions. We would like to thank the anonymous referees for their useful remarks that led to important improvements and a better presentation of this paper.

References


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<td>6400</td>
<td>1.4783(+2)</td>
<td>2.0797(-3)</td>
<td>2.0797(-3)</td>
<td>2.0797(-3)</td>
<td>2.0797(-3)</td>
<td>1.00</td>
<td></td>
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</tbody>
</table>

Table 2. Estimator $E_\varepsilon^L(T)$ at $t = 1.0$ with $\varepsilon = 0.01$, and rates of convergence.

<table>
<thead>
<tr>
<th>$k^{-1}$</th>
<th>$h^{-1} = 32$</th>
<th>$h^{-1} = 64$</th>
<th>$h^{-1} = 128$</th>
<th>$h^{-1} = 256$</th>
<th>$h^{-1} = 512$</th>
<th>$h^{-1} = 1024$</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.4779(+2)</td>
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<td>9.9966(-4)</td>
<td>9.9966(-4)</td>
<td>9.9966(-4)</td>
<td>9.9966(-4)</td>
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</tr>
<tr>
<td>200</td>
<td>1.4788(+2)</td>
<td>2.4993(-4)</td>
<td>2.4993(-4)</td>
<td>2.4993(-4)</td>
<td>2.4993(-4)</td>
<td>2.00</td>
<td></td>
</tr>
<tr>
<td>400</td>
<td>1.4787(+2)</td>
<td>6.2482(-5)</td>
<td>6.2482(-5)</td>
<td>6.2482(-5)</td>
<td>6.2482(-5)</td>
<td>2.00</td>
<td></td>
</tr>
<tr>
<td>800</td>
<td>1.4787(+2)</td>
<td>1.5621(-5)</td>
<td>1.5621(-5)</td>
<td>1.5621(-5)</td>
<td>1.5621(-5)</td>
<td>2.00</td>
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</tr>
<tr>
<td>1600</td>
<td>1.4787(+2)</td>
<td>3.9052(-6)</td>
<td>3.9052(-6)</td>
<td>3.9052(-6)</td>
<td>3.9052(-6)</td>
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</tr>
<tr>
<td>3200</td>
<td>1.4787(+2)</td>
<td>9.7629(-7)</td>
<td>9.7629(-7)</td>
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<tr>
<td>6400</td>
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<td>2.4407(-7)</td>
<td>2.4407(-7)</td>
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</tr>
</tbody>
</table>

Table 3. Estimator $E_\varepsilon^S(T)$ at $t = 1.0$ with $\varepsilon = 0.001$, and rates of convergence.

<table>
<thead>
<tr>
<th>$k^{-1}$</th>
<th>$h^{-1} = 128$</th>
<th>$h^{-1} = 256$</th>
<th>$h^{-1} = 512$</th>
<th>$h^{-1} = 1024$</th>
<th>Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>5.0586(+2)</td>
<td>1.3104(-1)</td>
<td>1.3104(-1)</td>
<td>1.3104(-1)</td>
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</tr>
<tr>
<td>800</td>
<td>5.0586(+2)</td>
<td>6.5526(-2)</td>
<td>6.5526(-2)</td>
<td>6.5526(-2)</td>
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<tr>
<td>1600</td>
<td>5.0586(+2)</td>
<td>3.2764(-2)</td>
<td>3.2764(-2)</td>
<td>3.2764(-2)</td>
<td>1.00</td>
</tr>
<tr>
<td>3200</td>
<td>5.0586(+2)</td>
<td>1.6382(-2)</td>
<td>1.6382(-2)</td>
<td>1.6382(-2)</td>
<td>1.00</td>
</tr>
<tr>
<td>6400</td>
<td>5.0586(+2)</td>
<td>8.1911(-3)</td>
<td>8.1911(-3)</td>
<td>8.1911(-3)</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Table 4. Estimator $E_\varepsilon^L(T)$ at $t = 1.0$ with $\varepsilon = 0.0025$, and rates of convergence.
\[ h^{-1} = 128 \quad h^{-1} = 256 \quad h^{-1} = 512 \quad h^{-1} = 1024 \quad \text{Rate} \]

<table>
<thead>
<tr>
<th>( k^{-1} )</th>
<th>( h^{-1} = 128 )</th>
<th>( h^{-1} = 256 )</th>
<th>( h^{-1} = 512 )</th>
<th>( h^{-1} = 1024 )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>5.0586(2)</td>
<td>2.4582(-4)</td>
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<td>2.4582(-4)</td>
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<tr>
<td>800</td>
<td>5.0586(2)</td>
<td>6.1455(-5)</td>
<td>6.1455(-5)</td>
<td>6.1455(-5)</td>
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<tr>
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<td>1.5364(-5)</td>
<td>1.5364(-5)</td>
<td>1.5364(-5)</td>
</tr>
<tr>
<td>3200</td>
<td>5.0586(2)</td>
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<td>3.8410(-6)</td>
<td>3.8410(-6)</td>
</tr>
<tr>
<td>6400</td>
<td>5.0586(2)</td>
<td>9.6024(-7)</td>
<td>9.6024(-7)</td>
<td>9.6024(-7)</td>
</tr>
</tbody>
</table>

Table 5. Estimator \( \xi_n^E(T) \) at \( t = 1.0 \) with \( \varepsilon = 0.0025 \), and rates of convergence.