A New Finite Volume Scheme for a Linear Schrödinger Evolution Equation

Abdallah Bradji

Abstract We consider the linear Schrödinger evolution equation with a time dependent potential in several space dimension. We provide a new implicittime finite volume scheme, using the general nonconforming meshes of [2] as discretization in space. We prove that the convergence order is $h_{\mathscr{D}}+k$, where $h_{\mathscr{D}}$ (resp. k) is the mesh size of the spatial (resp. time) discretization, in discrete norms $\mathbb{L}^\infty(0, T; H_0^1(\Omega))$ and $\mathscr{W}^{1,\infty}(0, T; L^2(\Omega))$. These error estimates are useful because they allow to obtain approximations to the exact solution and its first derivatives of order $h_{\mathscr{D}}+k$.

1 Motivation and Aim of This Paper

Let us consider the following linear time dependent Schrödinger problem. We seek a complex valued function u defined on $\Omega \times [0, T]$ satisfying

$$i\, u_t(x,t) + \Delta u(x,t) - V(x,t)u(x,t) = f(x,t), \;\; (x,t) \in \Omega \times (0,T), \tag{1}$$

where Ω is an open bounded polyhedral subset in $\mathbb{R}^d$, with $d \in \mathbb{N} \setminus \{0\}$, $T > 0$, $i \in \mathbb{C}$ (the set of complex numbers) is the imaginary unit, V is a time dependent potential and f is a given function.

An initial condition is given by:

$$u(x,0) = u^0(x), \;\; x \in \Omega, \tag{2}$$

A. Bradji(✉)
Department of Mathematics, Faculty of Sciences, University of Badji Mokhtar-Annaba, Annaba, Algeria
e-mail: abdallah-bradji@univ-annaba.org, bradji@cmi.univ-mrs.fr

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with homogeneous Dirichlet boundary conditions, that is

$$u(x,t) = 0, \ \ (x,t) \in \partial\Omega \times (0,T), \tag{3}$$

The form (1)–(3) of Schrödinger equation occurs, for example, when $d = 1$ in underwater acoustics, cf. [1]. The model (1)–(3) is studied for instance in [1] when a Galerkin finite element method is used as discretization in space. The stationary case of Schrödinger equation is also considered using finite volume methods in [3] where there are some interesting numerical tests. In this work we analyze a new finite volume scheme for the Schrödinger evolution problem (1)–(3).

2 Definition of the Scheme and Statement of the Main Result

The discretization of Ω is performed using the mesh $\mathscr{D} = (\mathscr{M}, \mathscr{E}, \mathscr{P})$ described in [2, Definition 2.1] which we recall here for the sake of completeness.

Definition 1 (Definition of the spatial mesh) Let Ω be a polyhedral open bounded subset of $\mathbb{R}^d$, where $d \in \mathbb{N} \setminus \{0\}$, and $\partial\Omega = \overline{\Omega} \setminus \Omega$ its boundary. A discretisation of Ω, denoted by $\mathscr{D}$, is defined as the triplet $\mathscr{D} = (\mathscr{M}, \mathscr{E}, \mathscr{P})$, where:

1. $\mathscr{M}$ is a finite family of non empty connected open disjoint subsets of Ω (the "control volumes") such that $\overline{\Omega} = \cup_{K\in\mathscr{M}}\overline{K}$. For any $K \in \mathscr{M}$, let $\partial K = \overline{K} \setminus K$ be the boundary of K; let $\mathrm{m}(K) > 0$ denote the measure of K and h_K denote the diameter of K.
2. $\mathscr{E}$ is a finite family of disjoint subsets of $\overline{\Omega}$ (the "edges" of the mesh), such that, for all $\sigma \in \mathscr{E}$, σ is a non empty open subset of a hyperplane of $\mathbb{R}^d$, whose $(d-1)$–dimensional measure is strictly positive. We also assume that, for all $K \in \mathscr{M}$, there exists a subset $\mathscr{E}_K$ of $\mathscr{E}$ such that $\partial K = \cup_{\sigma\in\mathscr{E}_K}\overline{\sigma}$. For any $\sigma \in \mathscr{E}$, we denote by $\mathscr{M}_\sigma = \{K; \ \sigma \in \mathscr{E}_K\}$. We then assume that, for any $\sigma \in \mathscr{E}$, either $\mathscr{M}_\sigma$ has exactly one element and then $\sigma \subset \partial\Omega$ (the set of these interfaces, called boundary interfaces, denoted by $\mathscr{E}_{\mathrm{ext}}$) or $\mathscr{M}_\sigma$ has exactly two elements (the set of these interfaces, called interior interfaces, denoted by $\mathscr{E}_{\mathrm{int}}$). For all $\sigma \in \mathscr{E}$, we denote by x_σ the barycentre of σ. For all $K \in \mathscr{M}$ and $\sigma \in \mathscr{E}$, we denote by $\mathbf{n}_{K,\sigma}$ the unit vector normal to σ outward to K.
3. $\mathscr{P}$ is a family of points of Ω indexed by $\mathscr{M}$, denoted by $\mathscr{P} = (x_K)_{K\in\mathscr{M}}$, such that for all $K \in \mathscr{M}$, $x_K \in K$ and K is assumed to be x_K–star-shaped, which means that for all $x \in K$, the property $[x_K, x] \subset K$ holds. Denoting by $d_{K,\sigma}$ the Euclidean distance between x_K and the hyperplane including σ, one assumes that $d_{K,\sigma} > 0$. We then denote by $\mathscr{D}_{K,\sigma}$ the cone with vertex x_K and basis σ.

The time discretization is performed with a constant time step $k = \frac{T}{N+1}$, where $N \in \mathbb{N}^\star$, and we shall denote $t_n = nk$, for $n \in [\![0, N+1]\!]$. Throughout this paper, the letter C stands for a positive constant independent of the parameters of the space and time discretizations and its values may be different in different appearance.

Since we deal with a complex valued solution, one has to seek for an approximation in discrete spaces over the field of complex numbers $\mathbb{C}$. Some slight modifications should be made on the discrete spaces used in [2]. In particular, we define the space $\mathcal{X}_{\mathcal{D}}$ as the set of all $\left((v_K)_{K\in\mathcal{M}},\ (v_\sigma)_{\sigma\in\mathcal{E}}\right)$, where $v_K, v_\sigma \in \mathbb{C}$ for all $K \in \mathcal{M}$ and for all $\sigma \in \mathcal{E}$, and $\mathcal{X}_{\mathcal{D},0} \subset \mathcal{X}_{\mathcal{D}}$ is the set of all $v \in \mathcal{X}_{\mathcal{D}}$ such that $v_\sigma = 0$ for all $\sigma \in \mathcal{E}_{\text{ext}}$. Let $H_{\mathcal{M}}(\Omega, \mathbb{C})$ be the space of functions from Ω to $\mathbb{C}$ which are constant over each control volume of the mesh. For all $v \in \mathcal{X}_{\mathcal{D}}$, we denote by $\Pi_{\mathcal{M}}\, v \in H_{\mathcal{M}}(\Omega, \mathbb{C})$ the function defined by $\Pi_{\mathcal{M}}\, v(x) = v_K$, for a.e. $x \in K$, for all $K \in \mathcal{M}$.

For all $\varphi \in \mathcal{C}(\Omega, \mathbb{C})$, we define $\mathcal{P}_{\mathcal{D}}\varphi = \left((\varphi(x_K))_{K\in\mathcal{M}},\ (\varphi(x_\sigma))_{\sigma\in\mathcal{E}}\right) \in \mathcal{X}_{\mathcal{D}}$. We denote by $\mathcal{P}_{\mathcal{M}}\varphi \in H_{\mathcal{M}}(\Omega, \mathbb{C})$ the function defined by $\mathcal{P}_{\mathcal{M}}\,\varphi(x) = \varphi(x_K)$, for a.e. $x \in K$, for all $K \in \mathcal{M}$. We will use the norm $\|\cdot\|_{1,2,\mathcal{M}}$ given by [2, (4.5), p. 1026].

In order to analyze the convergence, we need to consider the size of the discretization $\mathcal{D}$ defined by $h_{\mathcal{D}} = \sup\{\text{diam(K)},\ K \in \mathcal{M}\}$ and the regularity of the mesh given by $\theta_{\mathcal{D}} = \max\left(\max_{\sigma\in\mathcal{E}_{\text{int}},K,L\in\mathcal{M}} \dfrac{d_{K,\sigma}}{d_{L,\sigma}},\ \max_{K\in\mathcal{M},\sigma\in\mathcal{E}_K} \dfrac{h_K}{d_{K,\sigma}}\right)$.

The scheme we want to consider in this note is based on the use of the discrete gradient given in [2]. For $u \in \mathcal{X}_{\mathcal{D}}$, we define, for all $K \in \mathcal{M}$

$$\nabla_{\mathcal{D}}\, u(x) = \nabla_{K,\sigma}\, u, \quad \text{a. e. } x \in \mathcal{D}_{K,\sigma}, \tag{4}$$

where $\mathcal{D}_{K,\sigma}$ is the cone with vertex x_K and basis σ and

$$\nabla_{K,\sigma} u = \nabla_K\, u + \left(\frac{\sqrt{d}}{d_{K,\sigma}}\left(u_\sigma - u_K - \nabla_K\, u \cdot (x_\sigma - x_K)\right)\right)\mathbf{n}_{K,\sigma}, \tag{5}$$

where $\nabla_K\, u = \dfrac{1}{\text{m}(K)} \displaystyle\sum_{\sigma\in\mathcal{E}_K} \text{m}(\sigma)\,(u_\sigma - u_K)\,\mathbf{n}_{K,\sigma}$ and d is the space dimension.

We define the finite volume approximation for (1)–(3) as $\left(u^n_{\mathcal{D}}\right)_{n=0}^{N+1} \in \mathcal{X}_{\mathcal{D},0}^{N+2}$ with $u^n_{\mathcal{D}} = \left(\left(u^n_K\right)_{K\in\mathcal{M}},\left(u^n_\sigma\right)_{\sigma\in\mathcal{E}}\right)$, for all $n \in \{0, \ldots, N+1\}$ and

1. discretization of the initial conditions (2): for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\langle u^0_{\mathcal{D}}, v\rangle_F + \left(V(0)\Pi_{\mathcal{M}}\, u^0_{\mathcal{D}}, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)} = \left(-\Delta\, u^0 + V(0)u^0, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)}, \tag{6}$$

2. discretization of Eq. (1): for any $n \in \{1, \ldots, N\}$, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$\begin{aligned} &i\left(\partial^1\, \Pi_{\mathcal{M}}\, u^{n+1}_{\mathcal{D}}, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)} - \langle u^{n+1}_{\mathcal{D}}, v\rangle_F - \left(V(t_{n+1})\Pi_{\mathcal{M}}\, u^{n+1}_{\mathcal{D}}, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)} \\ &\quad = \left(\frac{1}{k}\int_{t_n}^{t_{n+1}} f(t)dt, \Pi_{\mathcal{M}}\, v\right)_{\mathbb{L}^2(\Omega)}, \end{aligned} \tag{7}$$

where $\langle u, v\rangle_F = \int_\Omega \nabla_{\mathscr{D}} u(x)\cdot\nabla_{\mathscr{D}} \bar{v}(x)dx$, $\partial^1 v^n = \dfrac{v^n - v^{n-1}}{k}$, and $(\cdot,\cdot)_{\mathbb{L}^2(\Omega)}$ denotes the $\mathbb{L}^2$-inner product of the space $\mathbb{L}^2(\Omega,\mathbb{C})$.

The main result of the present contribution is the following theorem.

Theorem 1 (Error estimates for the finite volume scheme (6)– (7)) *Let Ω be a polyhedral open bounded subset of $\mathbb{R}^d$, where $d \in \mathbb{N}\setminus\{0\}$, and $\partial\Omega = \overline{\Omega}\setminus\Omega$ its boundary. Assume that the solution of the Schrödinger evolution problem of (1)–(3) satisfies $u \in \mathscr{C}^2([0,T];\ \mathscr{C}^2(\overline{\Omega},\mathbb{C}))$ and the time dependent potential V is satisfying $V \in \mathscr{C}([0,T];\ \mathbb{L}^\infty(\Omega,\mathbb{R}))$ and $V(t)(x) \ge 0$ for all $t\in[0,T]$ and for a.e. $x\in\Omega$. Let $k = \frac{T}{N+1}$, with $N \in \mathbb{N}^\star$, and denote by $t_n = nk$, for $n\in\{0,\ldots,N+1\}$. Let $\mathscr{D} = (\mathscr{M},\mathscr{E},\mathscr{P})$ be a discretization in the sense of [2, Definition 2.1]. Assume that $\theta_{\mathscr{D}}$ satisfies $\theta \ge \theta_{\mathscr{D}}$.*

Then there exists a unique solution $\left(u_{\mathscr{D}}^n\right)_{n=0}^{N+1} \in \mathscr{X}_{\mathscr{D},0}^{N+2}$ for problem (6)–(7). Assume in addition that $V \in \mathscr{C}^j([0,T];\ \mathbb{L}^\infty(\Omega,\mathbb{R}))$ for all $j\in\{1,2\}$. Then, the following error estimates hold:

- *Discrete $\mathbb{L}^\infty(0,T;H_0^1(\Omega))$–estimate: for all $n\in\{0,\ldots,N+1\}$*

$$\|\mathscr{P}_{\mathscr{M}} u(t_n) - \Pi_{\mathscr{M}} u_{\mathscr{D}}^n\|_{1,2,\mathscr{M}} \le C(k+h_{\mathscr{D}})\|u\|_{\mathscr{C}^2([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \tag{8}$$

- *Discrete $\mathscr{W}^{1,\infty}(0,T;\mathbb{L}^2(\Omega))$–estimate: for all $n\in\{1,\ldots,N+1\}$*

$$\|\partial^1(\mathscr{P}_{\mathscr{M}} u(t_n) - \Pi_{\mathscr{M}} u_{\mathscr{D}}^n)\|_{\mathbb{L}^2(\Omega)} \le C(k+h_{\mathscr{D}})\|u\|_{\mathscr{C}^2([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \tag{9}$$

- *Error estimate in the gradient approximation: for all $n\in\{0,\ldots,N+1\}$*

$$\|\nabla_{\mathscr{D}} u_{\mathscr{D}}^n - \nabla u(t_n)\|_{\mathbb{L}^2(\Omega)} \le C(k+h_{\mathscr{D}})\|u\|_{\mathscr{C}^2([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \tag{10}$$

The following lemma will help us to prove Theorem 1:

Lemma 1 (A new a priori estimate) *We consider the same discretizations as in Theorem 1. Assume that $\theta_{\mathscr{D}}$ satisfies $\theta\ge\theta_{\mathscr{D}}$ and that there exists $\left(\eta_{\mathscr{D}}^n\right)_{n=0}^{N+1} \in \mathscr{X}_{\mathscr{D},0}^{N+2}$ such that $\eta_{\mathscr{D}}^0 = 0$ and for any $n\in\{0,\ldots,N\}$, for all $v\in\mathscr{X}_{\mathscr{D},0}$*

$$\begin{aligned} i\left(\Pi_{\mathscr{M}}\partial^1\eta_{\mathscr{D}}^{n+1}, \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)} - \langle\eta_{\mathscr{D}}^{n+1}, v\rangle_F - \left(V(t_{n+1})\Pi_{\mathscr{M}}\eta_{\mathscr{D}}^{n+1}, \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)} \\ = \left(\mathscr{S}^n, \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)}, \end{aligned} \tag{11}$$

where $\mathscr{S}^n \in \mathbb{L}^2(\Omega,\mathbb{C})$, for all $n\in\{0,\ldots,N\}$ and $V\in\mathscr{C}([0,T];\ \mathbb{L}^\infty(\Omega,\mathbb{R}))$ satisfying $V(t)(x)\ge 0$ for all $t\in[0,T]$ and for a.e. $x\in\Omega$. Assume in addition that $V\in\mathscr{C}^j([0,T];\ \mathbb{L}^\infty(\Omega,\mathbb{R}))$ for all $j\in\{1,2\}$. Then the following estimate holds, for all $j\in\{0,\ldots,N\}$

$$\begin{aligned}&\| \Pi_{\mathcal{M}}\, \partial^1\, \eta_{\mathcal{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)} + \| \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^{j+1} \|_{1,2,\mathcal{M}} + \| \nabla_{\mathcal{D}}\, \eta_{\mathcal{D}}^{j+1} \|_{(\mathbb{L}^2(\Omega))^d}\\ &\leq C(\mathcal{S} + \mathcal{S}_1),\end{aligned} \tag{12}$$

where $\mathcal{S} = \max_{n=0}^{N} \| \mathcal{S}^n \|_{\mathbb{L}^2(\Omega)}$ *and* $\mathcal{S}_1 = \max_{n=1}^{N} \| \partial^1 \mathcal{S}^n \|_{\mathbb{L}^2(\Omega)}$.

Proof **1. Estimate on** $\| \Pi_{\mathcal{M}}\, \partial^1\, \eta_{\mathcal{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)}$. Acting the discrete operator ∂^1 on both sides of (11) and using the formula $\partial^1(r^n s^n) = s^n \partial^1 r^n + r^{n-1}\partial^1 s^n$ yields

$$\begin{aligned}&i \left(\Pi_{\mathcal{M}}\, \partial^2\, \eta_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)} - \langle \partial^1 \eta_{\mathcal{D}}^{n+1}, v \rangle_F - \left(V(t_{n+1}) \partial^1 \Pi_{\mathcal{M}}\, \eta_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)}\\ &= \left(\partial^1 \mathcal{S}^n, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)} + \left(\partial^1 V(t_{n+1}) \Pi_{\mathcal{M}}\, \eta_{\mathcal{D}}^n, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)}.\end{aligned} \tag{13}$$

Choosing $v = \partial^1 \eta_{\mathcal{D}}^{n+1}$ in (13) and taking the imaginary part of the result, we get

$$\begin{aligned}&\mathrm{Re} \left(\Pi_{\mathcal{M}}\, \partial^2\, \eta_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)}\\ &= \mathrm{Im} \left(\left(\partial^1 \mathcal{S}^n, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)} + \left(\partial^1 V(t_{n+1}) \Pi_{\mathcal{M}}\, \eta_{\mathcal{D}}^n, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)} \right).\end{aligned} \tag{14}$$

Some calculations lead to the expression, for all function $(\omega^n)_{n=0}^{N+1} \in (\mathbb{L}^2(\Omega, \mathbb{C}))^{N+2}$:

$$\begin{aligned}2k \left(\partial^1\, \omega^{n+1}, \omega^{n+1} \right)_{\mathbb{L}^2(\Omega)} =& \| \omega^{n+1} - \omega^n \|_{\mathbb{L}^2(\Omega)}^2\\ &+ \| \omega^{n+1} \|_{\mathbb{L}^2(\Omega)}^2 - \| \omega^n \|_{\mathbb{L}^2(\Omega)}^2 + 2i\, \mathrm{Im} \left(\omega^{n+1}, \omega^n \right)_{\mathbb{L}^2(\Omega)}\end{aligned} \tag{15}$$

Gathering (14) with (15) when $\omega^{n+1} = \Pi_{\mathcal{M}} \partial^1 \eta_{\mathcal{D}}^{n+1}$, using the fact that $V \in \mathcal{C}^1([0, T];\ \mathbb{L}^\infty(\Omega, \mathbb{R}))$, and the Cauchy Schwarz inequality, we get

$$\begin{aligned}&\| \Pi_{\mathcal{M}} \partial^1 \eta_{\mathcal{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}^2 - \| \Pi_{\mathcal{M}} \partial^1 \eta_{\mathcal{D}}^n \|_{\mathbb{L}^2(\Omega)}^2\\ &\leq 2kC(\mathcal{S}_1 + \| \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^n \|_{\mathbb{L}^2(\Omega)}) \| \Pi_{\mathcal{M}} \partial^1 \eta_{\mathcal{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}.\end{aligned} \tag{16}$$

Let us prove an $\mathbb{L}^\infty(0, T;\ \mathbb{L}^2(\Omega, \mathbb{C}))$-estimate. Taking $v = \eta_{\mathcal{D}}^{n+1}$ in (11) and using the fact that V is a real valued function, and taking the imaginary part to get

$$\mathrm{Re} \left(\Pi_{\mathcal{M}}\, \partial^1\, \eta_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}}\, \eta_{\mathcal{D}}^{n+1} \right)_{\mathbb{L}^2(\Omega)} = \mathrm{Im} \left(\mathcal{S}^n, \Pi_{\mathcal{M}}\, v \right)_{\mathbb{L}^2(\Omega)}. \tag{17}$$

This with (15) when $\omega^{n+1} = \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^{n+1}$, and the Cauchy Schwarz inequality yields

$$\| \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}^2 - \| \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^n \|_{\mathbb{L}^2(\Omega)}^2 \leq 2k\mathcal{S} \| \Pi_{\mathcal{M}} \eta_{\mathcal{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}. \tag{18}$$

Summing (18) over $n \in \{0, \ldots, j\}$, where $j \in \{0, \ldots, N\}$, and using the fact $\eta_{\mathscr{D}}^0 = 0$ yields $\| \Pi_{\mathscr{M}} \eta_{\mathscr{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)}^2 \leq 2k\mathscr{S} \sum_{n=0}^{j} \| \Pi_{\mathscr{M}} \eta_{\mathscr{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}$. Applying a Young's inequality (as applied in (20) below) and using the discrete Gronwall's lemma yields

$$\| \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)} \leq C\mathscr{S}. \tag{19}$$

Inserting this estimate in (16) and summing the result over $n \in \{1, \ldots, j\}$, where $j \in \{1, \ldots, N\}$ yields

$$\begin{aligned}
&\| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)}^2 - \| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{1} \|_{\mathbb{L}^2(\Omega)}^2 \\
&\qquad \leq 2kC(\mathscr{S} + \mathscr{S}_1) \sum_{n=1}^{j} \| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{n+1} \|_{\mathbb{L}^2(\Omega)}.
\end{aligned}$$

This with a Young's inequality leads to

$$\begin{aligned}
\| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{j+1} \|_{\mathbb{L}^2(\Omega)}^2 \leq \frac{2k}{T} \sum_{n=2}^{j} \| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{n} \|_{\mathbb{L}^2(\Omega)}^2 + 2 \| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{1} \|_{\mathbb{L}^2(\Omega)}^2 \\
+ 8T^2\, (C)^2\, (\mathscr{S} + \mathscr{S}_1)^2 .
\end{aligned} \tag{20}$$

We now estimate $\| \Pi_{\mathscr{M}} \partial^1 \eta_{\mathscr{D}}^{1} \|_{\mathbb{L}^2(\Omega,\mathbb{C})}^2$. To this end, we set $n = 0$ and $v = \partial^1\, \eta_{\mathscr{D}}^1$ in (11) and we use the fact that $\partial^1\, \eta_{\mathscr{D}}^1 = \dfrac{\eta_{\mathscr{D}}^1}{k}$ (this stems from $\eta_{\mathscr{D}}^0 = 0$)

$$\begin{aligned}
i \| \Pi_{\mathscr{M}}\, \partial^1\, \eta_{\mathscr{D}}^1 \|_{\mathbb{L}^2(\Omega)}^2 - \frac{1}{k} \langle \eta_{\mathscr{D}}^1, \eta_{\mathscr{D}}^1 \rangle_F - \frac{1}{k} \Big(V(t_1) \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^1, \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^1 \Big)_{\mathbb{L}^2(\Omega)} \\
= \Big(\mathscr{S}^0, \Pi_{\mathscr{M}}\, \partial^1\, \eta_{\mathscr{D}}^1 \Big)_{\mathbb{L}^2(\Omega)} .
\end{aligned} \tag{21}$$

Taking the imaginary part in (21) and using the Cauchy Schwarz inequality implies $\| \Pi_{\mathscr{M}}\, \partial^1\, \eta_{\mathscr{D}}^1 \|_{\mathbb{L}^2(\Omega)} \leq \mathscr{S}$. This with inequality (20) and the discrete version of the Gronwall's lemma yields the desired estimate $\mathscr{W}^{1,\infty}(0, T;\ \mathbb{L}^2)$-estimate in (12).

2. Estimate on $\| \Pi_{\mathscr{M}} \eta_{\mathscr{D}}^{j+1} \|_{1,2,\mathscr{M}}$. Choosing $v = \partial^1 \eta_{\mathscr{D}}^{n+1}$ in (11) and taking the real part yields

$$\begin{aligned}
\mathrm{Re} \left(\langle \eta_{\mathscr{D}}^{n+1}, \partial^1 \eta_{\mathscr{D}}^{n+1} \rangle_F + \Big(V(t_{n+1}) \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}, \partial^1 \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1} \Big)_{\mathbb{L}^2(\Omega)} \right) \\
= \mathrm{Re} \left(-\mathscr{S}^n, \Pi_{\mathscr{M}}\, v \right)_{\mathbb{L}^2(\Omega)} .
\end{aligned} \tag{22}$$

Writing $\langle \eta_{\mathscr{D}}^{n+1}, \partial^1 \eta_{\mathscr{D}}^{n+1}\rangle_F$ and $\left(V(t_{n+1})\Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}, \partial^1 \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}\right)_{\mathbb{L}^2(\Omega)}$ in a similar manner to that of (15) and gathering this with (22) leads to

$$\begin{aligned}\langle \eta_{\mathscr{D}}^{n+1}, \eta_{\mathscr{D}}^{n+1}\rangle_F - \langle \eta_{\mathscr{D}}^{n}, \eta_{\mathscr{D}}^{n}\rangle_F + \left(V(t_{n+1})\Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}, \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}\right)_{\mathbb{L}^2(\Omega)} \\ - \left(V(t_{n+1})\Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n}, \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n}\right)_{\mathbb{L}^2(\Omega)} \\ \le 2k \,\mathrm{Re}\left(-\mathscr{S}^n, \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)}.\end{aligned} \tag{23}$$

Summing (23) over $n \in \{0, \ldots, j\}$, where $j \in \{0, \ldots, N\}$, using the Cauchy Schwarz inequality and [2, Lemma 4.2] yields $|\eta_{\mathscr{D}}^{j+1}|_{\mathscr{X}}^2 \le Ck\mathscr{S}\sum_{n=0}^{j} \| \partial^1 \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}\|_{\mathbb{L}^2(\Omega)}$. This with the estimate on $\|\Pi_{\mathscr{M}}\, \partial^1 \eta_{\mathscr{D}}^{j+1}\|_{\mathbb{L}^2(\Omega)}$ (it is proved in in the previous item) yields

$$|\eta_{\mathscr{D}}^{j+1}|_{\mathscr{X}} \le C(\mathscr{S} + \mathscr{S}_1). \tag{24}$$

This with the inequality norm [2, (4.6), p. 1026] implies the desired estimate $\mathbb{L}^\infty(0, T;\ H^1(\Omega))$-estimate in (12).

3. Estimate $\| \nabla_{\mathscr{D}}\, \eta_{\mathscr{D}}^{j+1}\|_{(\mathbb{L}^2(\Omega))^d}$. Estimate (24) with [2, Lemma 4.2] implies the estimate concerning $\| \nabla_{\mathscr{D}}\, \eta_{\mathscr{D}}^{j+1}\|_{(\mathbb{L}^2(\Omega))^d}$ in (12). ∎

Sketch of the proof of Theorem 1: The uniqueness of $\left(u_{\mathscr{D}}^n\right)_{n\in\{0,\ldots,N+1\}}$ satisfying (6)–(7) can be deduced using the [2, Lemma 4.2]. As usual, we use this uniqueness to prove the existence. To prove the error estimates (8)–(10), we compare the solution $u_{\mathscr{D}}^n$ with the solution: for any $n \in \{0, \ldots, N+1\}$, find $\hat{u}_{\mathscr{D}}^n \in \mathscr{X}_{\mathscr{D},0}$ such that

$$\begin{aligned}\langle \hat{u}_{\mathscr{D}}^n, v\rangle_F + \left(V(t_n)\Pi_{\mathscr{M}}\hat{u}_{\mathscr{D}}^n, \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)} \\ = (-\Delta\, u(t_n) + V(t_n)u(t_n), \Pi_{\mathscr{M}}\, v)_{\mathbb{L}^2(\Omega)}, \quad \forall v \in \mathscr{X}_{\mathscr{D},0}.\end{aligned} \tag{25}$$

Step 1: Comparison between u and $\hat{u}_{\mathscr{D}}^n$. Using techniques of the proof of [2, Theorem 4.8] yields, for all $v \in \mathscr{X}_{\mathscr{D},0}$

$$\begin{aligned}\left\langle \mathscr{P}_{\mathscr{D}}u(t_n) - \hat{u}_{\mathscr{D}}^n, v\right\rangle_F + \left(V(t_n)(\mathscr{P}_{\mathscr{M}}\, u(t_n) - \Pi_{\mathscr{M}}\hat{u}_{\mathscr{D}}^n), \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)} \\ = \sum_{K\in\mathscr{M}}\sum_{\sigma\in\mathscr{E}_K} \mathscr{R}_{K,\sigma}\left(u(t_n)\right)(\bar{v}_K - \bar{v}_\sigma) + \left(V(t_n)r\left(u(t_n)\right), \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)},\end{aligned} \tag{26}$$

where the expression $\mathbb{E}_{\mathscr{D}}\left(u(t_n)\right) = \left(\sum_{K\in\mathscr{M}}\sum_{\sigma\in\mathscr{E}_K} \frac{d_{K,\sigma}}{\mathrm{m}(\sigma)} \left|\mathscr{R}_{K,\sigma}\left(u(t_n)\right)\right|^2\right)^{\frac{1}{2}}$ is satisfying the estimate $\mathbb{E}_{\mathscr{D}}\left(u(t_n)\right) \le Ch_{\mathscr{D}}\| u\|_{\mathscr{C}([0,T];\ \mathscr{C}^2(\overline{\Omega}))}$ and $r(u) = \mathscr{P}_{\mathscr{M}}\, u - u$. Taking $v = \mathscr{P}_{\mathscr{D}}u(t_n) - \hat{u}_{\mathscr{D}}^n$ in (26) yields

$$\langle v, v\rangle_F + \left(V(t_n)\Pi_{\mathscr{M}} v, \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)} = \sum_{K\in\mathscr{M}} \sum_{\sigma\in\mathscr{E}_K} \mathscr{R}_{K,\sigma}\left(u(t_n)\right)(\bar{v}_K - \bar{v}_\sigma) + \left(V(t_n)r\left(u(t_n)\right), \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)}. \quad (27)$$

This with [2, Lemma 4.2], the Cauchy Schwarz inequality, the Sobolev inequality of [2, Lemma 5.4], and the inequality norm [2, (4.6), p. 1026] yields that

$$|\mathscr{P}_{\mathscr{D}}u(t_n) - \hat{u}^n_{\mathscr{D}}|_{\mathscr{X}} \le Ch_{\mathscr{D}}\|u\|_{\mathscr{C}([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \quad (28)$$

This with [2, (4.6), p. 1026], [2, Lemma 4.2], and [2, Lemma 4.4] implies the error estimate:

$$\|\mathscr{P}_{\mathscr{M}}u(t_n) - \Pi_{\mathscr{M}}\hat{u}^n_{\mathscr{D}}\|_{1,2,\mathscr{M}} + \|\nabla u(t_n) - \nabla_{\mathscr{D}}\hat{u}^n\|_{\mathbb{L}^2(\Omega)} \le Ch_{\mathscr{D}}\|u\|_{\mathscr{C}([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \quad (29)$$

We will now derive an $\mathscr{W}^{1,\infty}(0,T;\mathbb{L}^2)$–estimate. Acting the discrete operator ∂^1 on Eq. (26) to get, for any $n \in \{1, \ldots, N+1\}$

$$\left\langle \partial^1\left(\mathscr{P}_{\mathscr{D}}u(t_n) - \hat{u}^n_{\mathscr{D}}\right), v\right\rangle_F + \left(V(t_n)\partial^1\left((\mathscr{P}_{\mathscr{M}}u(t_n) - \Pi_{\mathscr{M}}\hat{u}^n_{\mathscr{D}})\right), \Pi_{\mathscr{M}} v\right)_{\mathbb{L}^2(\Omega)} = \sum_{K\in\mathscr{M}} \sum_{\sigma\in\mathscr{E}_K} \mathscr{R}_{K,\sigma}\left(\partial^1 u(t_n)\right)(\bar{v}_K - \bar{v}_\sigma) + (\mathbb{T}_1 + \mathbb{T}_2 - \mathbb{T}_3, \Pi_{\mathscr{M}} v)_{\mathbb{L}^2(\Omega)}, \quad (30)$$

where $\mathbb{T}_1 = \partial^1\left(V(t_n)\right)(\mathscr{P}_{\mathscr{M}}u(t_n) - u(t_n))$, $\mathbb{T}_2 = V(t_{n-1})\partial^1\left((\mathscr{P}_{\mathscr{M}}u(t_n) - u(t_n))\right)$, and $\mathbb{T}_3 = \partial^1\left(V(t_n)\right)\left(\mathscr{P}_{\mathscr{M}}u(t_{n-1}) - \Pi_{\mathscr{M}}\hat{u}^{n-1}_{\mathscr{D}}\right)$. Thanks to Taylor expansions and $\mathbb{L}^\infty(0,T;H^1_0(\Omega))$-estimate in (29) with [2, Lemma 5.4], we have

$$\|\mathbb{T}_i\|_{\mathbb{L}^2(\Omega)} \le Ch_{\mathscr{D}}\|u\|_{\mathscr{C}^1([0,T];\ \mathscr{C}^2(\overline{\Omega}))}, \quad \forall i \in \{1,2,3\}. \quad (31)$$

Taking $v = \partial^1\left(\mathscr{P}_{\mathscr{D}}u(t_n) - \hat{u}^n_{\mathscr{D}}\right)$ in (30), using [2, Lemma 4.2], and gathering this with the Cauchy Schwarz inequality, [2, Lemma 5.4], [2, (4.6), p. 1026], and (31) to get

$$\|\partial^1\left(\mathscr{P}_{\mathscr{M}}u(t_n) - \Pi_{\mathscr{M}}\hat{u}^n_{\mathscr{D}}\right)\|_{\mathbb{L}^2(\Omega)} \le Ch_{\mathscr{D}}\|u\|_{\mathscr{C}^1([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \quad (32)$$

Using the same techniques followed in (30)–(32), we are able to prove

$$\|\partial^2\left(\mathscr{P}_{\mathscr{M}}u(t_n) - \Pi_{\mathscr{M}}\hat{u}^n_{\mathscr{D}}\right)\|_{\mathbb{L}^2(\Omega)} \le Ch_{\mathscr{D}}\|u\|_{\mathscr{C}^2([0,T];\ \mathscr{C}^2(\overline{\Omega}))}. \quad (33)$$

Step 2: Comparison between $\hat{u}^n_{\mathscr{D}}$ and $u^n_{\mathscr{D}}$. Writing (25) in the step $n+1$, summing the result with (7) and using (1) yields, for all $n \in \{0, \ldots, N\}$

$$i\left(\partial^1 \Pi_{\mathscr{M}}\, \eta_{\mathscr{D}}^{n+1}, \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)} - \langle\, \eta_{\mathscr{D}}^{n+1}, v\rangle_F - \left(V(t_{n+1})\Pi_{\mathscr{M}}\eta_{\mathscr{D}}^{n+1}, \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)}$$
$$= \left(\mathscr{S}^n, \Pi_{\mathscr{M}}\, v\right)_{\mathbb{L}^2(\Omega)}, \tag{34}$$

where $\eta_{\mathscr{D}}^n = u_{\mathscr{D}}^n - \hat{u}_{\mathscr{D}}^n$ and $\mathscr{S}^n$ is given by

$$\mathscr{S}^n = i\partial^1(u(t_{n+1}) - \Pi_{\mathscr{M}}\, \hat{u}_{\mathscr{D}}^{n+1}) + \frac{1}{k}\int_{t_n}^{t_{n+1}} \Delta\, u(t)dt - \Delta\, u(t_{n+1})$$
$$- \frac{1}{k}\int_{t_n}^{t_{n+1}} V(t)u(t)dt + V(t_{n+1})u(t_{n+1}). \tag{35}$$

Thanks to suitable Taylor expansions and (32)–(33), we are able to justify that $\mathscr{S} + \mathscr{S}_1 \le C(k + h_{\mathscr{D}})\|\, u\|_{\mathscr{C}^2([0,T];\, \mathscr{C}^2(\overline{\Omega}))}$, where $\mathscr{S}$ and $\mathscr{S}_1$ are defined in Lemma 1. In addition to this, $\eta_{\mathscr{D}}^0 = 0$ (it stems from (2)). One remarks that $\left(\eta_{\mathscr{D}}^n\right)_{n=0}^{N+1}$ is satisfying hypothesis of Lemma 1, one can apply estimate (12) of Lemma 1 to obtain

$$\|\Pi_{\mathscr{M}}\, \partial^1\, \eta_{\mathscr{D}}^{j+1}\|_{\mathbb{L}^2(\Omega)} + \|\, \Pi_{\mathscr{M}}\eta_{\mathscr{D}}^{j+1}\|_{1,2,\mathscr{M}} + \|\, \nabla_{\mathscr{D}}\, \eta_{\mathscr{D}}^{j+1}\|_{\left(\mathbb{L}^2(\Omega)\right)^d}$$
$$\le C(k + h_{\mathscr{D}})\|\, u\|_{\mathscr{C}^2([0,T];\, \mathscr{C}^2(\overline{\Omega}))}. \tag{36}$$

This with estimates (29) and (32) implies estimates of Theorem 1. ∎

3 Conclusion and a Perspective

We considered the linear Schrödinger evolution equation. A convergence analysis of a new finite volume scheme is provided. We plan to consider the case when the spatial spatial domain is not bounded and to use the absorbing boundary conditions.

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