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Abstract. We study the approximation by a Voronoi finite-volume scheme of the Gross-Pitaevskii equation with time-dependent potential in two and three dimensions. We perform an explicit splitting scheme for the time integration alongside a two-point flux approximation scheme in space. We rigorously analyze the error bounds relying on discrete uniform Sobolev inequalities. We also prove the convergence of the pseudo-vorticity of the wave function. We finally perform some numerical simulations to illustrate our theoretical results.

1. Introduction

Let Ω be an open bounded connected polygonal or polyhedral subset of $\mathbb{R}^d$ with $d = 2$ or 3 and with Lipchitz boundary $\partial\Omega$. For $T > 0$, we consider the Gross-Pitaevskii equation

$$i\partial_t\psi + \Delta\psi = |\psi|^2\psi + V(t,x)\psi \tag{GP}$$

in $(0,T)\times\Omega$ with homogeneous Dirichlet boundary conditions $\psi(t,x) = 0$ for $(t,x) \in (0,T)\times\partial\Omega$ and initial condition $\psi(0) = \psi_0$. Equation (GP) appears as a fundamental model to describe the evolution of Bose-Einstein condensates, a state of matter near absolute zero temperature whose dynamics can be described by a single wave function ψ. The time-dependent potential $V = V(t,x) \in \mathbb{R}$ then both act as a magnetic confining potential and a stirring perturbation induced by laser beams. When set to rotation in a strong confinement regime, Bose-Einstein condensates exhibit complex nonlinear phenomena such as quantum turbulence, which have drawn more and more attention from the scientific community over the last decades. In particular, the nucleation of vortices with a quantized circulation, which are related to superfluid properties, as well as their interactions, played an important role for irreversible energy transfer mechanisms in quantum turbulent fluids [26].

The recent developments of laser trapping and cooling has made BEC experiments very precise in a number of complex configurations with various geometries. On the other hand, numerical simulations are usually made on periodic fields to allow the use of the Fast Fourier Transform in order to retain spectral accuracy, or with finite differences [4] on square or cubic lattices. This motivates the development of new methods in order to efficiently simulate the Gross-Pitaevskii equation on more general geometries. Here we will only assume that Ω is an open bounded connected polygonal set, and we analyze a numerical scheme based on a finite volume approximation in space. We perform a Two-Point Flux Approximation (TFPA) finite volume scheme, which stands as a very popular method in numerous applications, as it is both straightforward to implement and robust. Note that to the best of the author's knowledge, this is the first contribution to the numerical analysis of a finite volume scheme in the context of nonlinear dispersive PDEs. Even in the case of

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linear Schrödinger equations, the only work we are aware of is the recent paper of Bradji [6], in the context of hybrid finite volume scheme on general nonconforming meshes.

Finite elements methods has also recently been developed for the simulation of quantum fluids, in particular with the works of Henning and Målqvist [17] on convex domains, with GPElab developed by Antoine and Duboscq [2, 3] or the toolbox developed by Vergez, Danaila, Auliac and Hecht [24] on the FreeFEM++ software. Finite element methods are based on variational formulas, and usually require an adequate functional framework that we avoid here with our finite volume approach.

For the time integration of equation (GP), we will perform a standard Lie-Trotter splitting scheme. Alongside Runge-Kutta methods, splitting schemes are fairly popular for the explicit numerical integration of nonlinear Schrödinger equation as pointed out in the review paper [1], and we refer to the seminal works of Lubich [18] and Gauckler [14]. In the context of geometric numerical integration [16], splitting methods has the advantage of being easy to implement and efficient in terms of memory cost, while naturally preserving some important invariant of the continuous equation, such as the mass conservation of the Gross-Pitaevskii equation

$$\|\psi(t)\|_{L^2(\Omega)} = \|\psi_0\|_{L^2(\Omega)}$$

for all $t \in \mathbb{R}$. Note that equation (GP) also satisfies the energy balance law

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) = \int_\Omega \partial_t V(t,x)|\psi(t,x)|^2 \mathrm{d}x$$

where

$$E(t) = \frac{1}{2}\|\nabla\psi\|^2_{L^2(\Omega)} + \frac{1}{2}\|\psi(t)\|^4_{L^4(\Omega)} + \int_\Omega V(t,x)|\psi(t,x)|^2 \mathrm{d}x.$$

In particular, if $V = 0$, the energy E is also conserved over time, and it is now a common feature that splitting methods nearly conserved such energy over long times, see for instance [12].

From the theoretical point of view, the only work dealing with the Cauchy problem of nonlinear Schrödinger with time dependent potential seems to be [7]. In particular this paper ensures the existence of a unique global solution of equation (GP) on the whole space $\mathbb{R}^d$ for $d \leq 3$, under the condition that $V(t,x)$ is real-valued, locally bounded in time and subquadratic in space. A particular emphasises is also made on the growth of Sobolev norms of the solution over time.

Throughout all this paper we make the following assumption on the potential:

$$V \in \mathcal{C}([0,T], H^5(\Omega)).$$

We also suppose that this assumption would reasonably induce global existence and unicity of a smooth solution $\psi \in \mathcal{C}([0,T], H^5(\Omega))$ with initial condition $\psi_0 \in H^5(\Omega)$ on the open bounded subset Ω of $\mathbb{R}^d$. Note that this H^5-regularity assumption is already reguired for splitting schemes with finite differences [4, Theorem 4.3.]. Following the notations from [18], we write

$$m_k \coloneqq \sup_{t\in[0,T]} \|\psi(t)\|_{H^k(\Omega)} \quad \text{for } k = 1, \dots, 5.$$

This paper is organized as follows. In section 2, we will recall some notations about finite volume schemes in order to state our main result Theorem 1. Section 3 introduces some useful discrete functional properties for the Hilbert space H^1_h. In section 4 we prove an error estimate for the semi-discretization in space of the linear free Schrödinger equation. Section 5 and section 6 are then both devoted to the proof of Theorem 1, with respectively the convergence analysis of the semi-discrete in time and the fully-discrete schemes. In section 7, we show the L^1-convergence of the pseudo-vorticity of the wave function, a quantity which is of interest for efficient detection of vortices. Finally, in section 8 we perform some numerical simulations to illustrate our results.

2. Discrete framework and main result

2.1. **Finite volume notations.** In order to perform a finite volume scheme on Voronoï meshes for the Gross-Pitaevskii equation (GP), we first need to set a choice of spatial discretization. To this end, we consider finite-volumes admissible meshes in the sense of the following definition, as introduced in the seminal book of Eymard, Gallouët and Herbin [10].

Definition 1. ***(Admissible finite volume mesh).*** *An admissible finite-volume mesh $\mathcal{T}$ of Ω (see Figure 1) is given by a family of open polygonal (if $d = 2$) or polyhedral (if $d = 3$) and convex subsets K of Ω, called control volumes of $\mathcal{T}$, satisfying the following properties:*

- $\overline{\Omega} = \bigcup_{K\in\mathcal{T}} \overline{K}$.
- *If $K, L \in \mathcal{T}$ with $K \neq L$ then* $\operatorname{int} K \cap \operatorname{int} L = \emptyset$.
- *If $K, L \in \mathcal{T}$, with $K \neq L$ then either the $(d-1)$-dimensional Lebesgue measure of $\overline{K} \cap \overline{L}$ is 0 or $\overline{K} \cap \overline{L}$ is the edge (if $d = 2$) or face (if $d = 3$) of the mesh denoted $\sigma = K|L$ separating the control volumes K and L.*
- *To each control volume $K \in \mathcal{T}$, we associate a point $x_K \in \overline{K}$ (called the center of K) such that if $K, L \in \mathcal{T}$ are two neighboring control volumes, the straight line between the centers x_K and x_L is orthogonal to $\sigma = K|L$.*

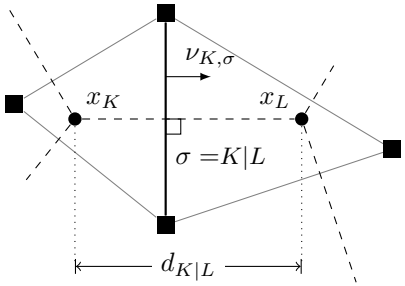

Figure 1. Notations of the mesh $\mathcal{T}$ associated with Ω.

In the case of *Voronoï meshes*, each control volume $K \in \mathcal{T}$ associated to a center x_K of the is defined by

$$K = \{x \in \Omega \mid |x - x_K| < |x - x_L|,\ \forall x_L \in \mathcal{T},\ x_L \neq x_K\}.$$

We denote by $h_K = \operatorname{diam}(K)$ for $K \in \mathcal{T}$, and

$$h \coloneqq \sup_{K\in\mathcal{T}} h_K$$

the mesh size of $\mathcal{T}$, as well as $d_h \in \mathbb{N}$ the number of control volumes $K \in \mathcal{T}$ of the finite-volume mesh. We also denote by $\mathcal{E}$ the set of edges/faces of the mesh $\mathcal{T}$, and we denote by e_h the number of edges in the mesh $\mathcal{T}$. We respectively define

$$\mathcal{E}_{\text{int}} \coloneqq \{\sigma \in \mathcal{E} \mid \sigma \notin \partial\Omega\} \quad \text{and} \quad \mathcal{E}_{\text{ext}} \coloneqq \{\sigma \in \mathcal{E} \mid \sigma \in \partial\Omega\}$$

the subsets of interior and exterior edges of $\mathcal{E}$. In the same vein, we denote by $\mathcal{E}_K$ the set of edges of any $K \in \mathcal{T}$, as well as $|K| \coloneqq \lambda_d(K)$ the area of the control volume K, where λ_d stands for the d-dimensional Lebesgue measure. In fact, regular Voronoï meshes often satisfy

$$\text{(boundary)} \qquad \mathcal{E}_K \cap \mathcal{E}_{\text{ext}} \neq \emptyset \Rightarrow x_K \in \partial\Omega,$$

a property that we will always assume in the following. Moreover, for K and L two neighboring control volumes of $\mathcal{T}$, we denote by $\sigma = K|L \in \mathcal{E}_{\rm int}$ their common edge, and by $|\sigma| = \lambda_{d-1}(\sigma)$ the length (for $d = 2$) or area (for $d = 3$) of σ. We also denote by $d_{K|L}$ the distance between x_K and x_L, and by $d_{K,\sigma}$ the length of the segment between x_K and σ, orthogonal to σ, if $\sigma \in \mathcal{E}_{\rm int}$. Once again, we refer to Figure 1 for an illustration of these notations in dimension $d = 2$. Note that in the case of (isotropic) Voronoï meshes, we have

$$d_{K,\sigma} = \frac{d_{K|L}}{2}, \quad \text{for } \sigma = K|L \in \mathcal{E}_{\rm int}, \tag{iso}$$

a property which will be useful in our upcoming analysis.

The use of the Voronoï method to produce admissible finite volume meshes goes back to the work of Mishev [20] and has now proven being powerful in a number of applications [13]. As pointed in [10, Example 9.2], an advantage of the Voronoï method is that it easily leads to meshes on non polygonal domain Ω, which might be of interest for physical applications. Note also that a relationship can be established between TPFA scheme on Voronoi meshes and generalized mixed-hybrid mimetic finite difference method, and super-convergence can occur [9].

In two dimension, a usual way to construct meshes satisfying the orthogonality property $(x_K, x_L) \perp \sigma$ is to partition Ω into a conforming triangulation with acute triangles called Delaunay triangulation, and to take each x_K as the circumcenter of K. This method is one of the most popular in computational mesh generation, and the dual mesh then corresponds to a Voronoï admissible finite volume mesh, leading to the use of *discrete duality finite volume* (DDFV) schemes [21]. Note that we will not exploit this duality property in the forthcoming analysis.

We will also assume the following regularity constraint on the mesh $\mathcal{T}$: there exists $0 < \xi < 1$ independent of h such that

$$h_K \xi \leq d_{K,\sigma} \leq h_K \quad \text{and} \quad h_K^{d-1} \xi \leq |\sigma| \leq h_K^{d-1} \tag{reg}$$

for any $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$. We define the following discrete norms:

Definition 2. ***(Discrete spaces).***
Let $U = (U_K)_K \in \mathbb{C}^{d_h}$ and $1 \leq p < \infty$. We define the L^p_h and L^∞_h norms of U by

$$\|U\|^p_{L^p_h} = \sum_{K\in\mathcal{T}} |K||U_K|^p \quad \textit{and} \quad \|U\|_{L^\infty_h} = \max_{K\in\mathcal{T}} |U_K|,$$

as well as the H^1_h semi-norm by

$$\|U\|^2_{H^1_h} = \sum_{\sigma\in\mathcal{E}_{\rm int}} \frac{|\sigma|}{d_{K|L}} |U_L - U_K|^2.$$

Note that the *discrete Poincaré inequality* (see [10, Lemma 9.1]) gives that

$$\|U\|_{L^2_h} \leq \operatorname{diam}(\Omega) \|U\|_{H^1_h},$$

so that the semi-norm $\|\cdot\|_{H^1_h}$ is in fact a norm. Finally we define the *pointwise evaluation operator* P_h of any continuous function $f \in \mathcal{C}(\Omega)$ by

$$(P_h f)_K = f(x_K) \quad \forall K \in \mathcal{T}.$$

2.2. **Splitting, finite volume scheme and main result.** Let $0 < \tau \leq 1$ be the time step size and $t_n = n\tau$ for $n \in \{0, \dots, N\}$ such that $T = N\tau$. We denote by $U^0 = P_h(\psi_0)$ the projection of the initial state ψ_0. We denote by A the matrix of the discrete Laplace operator defined for all $K \in \mathcal{T}$ by

$$(AU)_K = \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{E}_{\text{int}}} \frac{|\sigma|}{d_{K|L}} (U_L - U_K).$$

We also denote by

$$G_n(\tau, x) = \int_0^\tau V(t_n + s, x) \mathrm{d}s$$

the time antiderivative of V for all $x \in \Omega$, and we will assume that G_n can be evaluated exactly. We then define recursively our numerical scheme by a classical Lie-Trotter split-step

$$U^n = e^{i\tau A} e^{-iP_h G_n(\tau)} e^{-i\tau |U_{n-1}|^2} U^{n-1}, \quad U^0 = P_h(\psi_0), \tag{LT}$$

for $0 \leq n \leq N$, where multiplication between vectors of $\mathbb{C}^{d_h}$ has to be taken pointwise. We now state the main result of this work:

Theorem 1. *Let $\mathcal{T}$ be an admissible finite-volume Voronoï mesh of Ω satisfying the regularity properties (boundary)-(iso)-(reg). Let $\psi_0 \in H^5(\Omega)$ and $T > 0$. We assume that there exists a unique solution $\psi \in \mathcal{C}([0,T]; H^5(\Omega))$ of the Gross-Pitaevskii equation (GP) with $\psi(0) = \psi_0$. Let $U^0 = P_h\psi_0$, and we denote by $(U^n)_{0 \leq n \leq N}$ the sequence defined via the splitting method (LT). Then there exists $\tau_0 > 0$ and $h_0 > 0$ such that for $0 \leq n \leq N = T/\tau$, for all $0 < \tau \leq \tau_0$ and $0 < h \leq h_0$ satisfying the CFL-condition $\tau |\log h|^2 \leq 1$ for $d = 2$ or $\tau \leq h$ for $d = 3$, we have*

$$\|P_h\psi(t_n) - U^n\|_{H_h^1} \leq C(h + \tau),$$

where $C = C(m_5, T, \|V\|_{L_T^\infty H^5}, \varepsilon)$ and recalling that $m_5 = \sup_{t \in [0,T]} \|\psi(t)\|_{H^5(\Omega)}$.

We make the following comments:

- As mentionned in the introduction, this splitting scheme naturally preserves the L^2-norm of the solution
$$\|U^n\|_{L_h^2} = \|U^0\|_{L_h^2} \quad \forall 0 \leq n \leq N,$$
making the scheme (LT) unconditionnaly stable in L^2.
- One may also consider the Strang splitting scheme recursively defined by
$$U^n = e^{-i\frac{\tau}{2}|U_{n-1}|^2} e^{-iP_h G_{n+\frac{1}{2}}(\frac{\tau}{2})} e^{i\tau A} e^{-iP_h G_n(\frac{\tau}{2})} e^{-i\frac{\tau}{2}|U_{n-1}|^2} U^{n-1},$$
with $t_{n+\frac{1}{2}} = \frac{t_n + t_{n+1}}{2}$, taking advantage of computing once the Laplace operator part at each step (which will be the most costly from the finite volume perspective) along theoretically recovering a second order method in time which still preserves the L^2-norm of the initial state. Note however that the proof is more tedious so we omit it here. Higher order methods for the time discretization can thoroughly be considered, and we refer the interested reader to the book of Hairer, Lubich and Wanner [16].
- On the contrary, higher order methods for space discretization is generally a challenging task in the finite volume framework, and might be an interesting topic of research for future works.

We end this section with some notations. The $L^p(\Omega)$ and $H^k(\Omega)$ spaces will be written with the compact notation L^p and H^k in equation mode for conciseness purposes, as there is no ambiguity with the finite-dimensional spaces L_h^p and H_h^1. The same way, the uniform norm on a time interval

$[0,T]$ will be denoted $\|\cdot\|_{L^\infty_T}$. We also refer to *polygonal* control volumes K and *edges* σ as in the two-dimensional case $d=2$, even if it means *polyhedral* and *faces* for $d=3$. If not mention otherwise, an edge $\sigma \in \mathcal{E}_{\rm int}$ is systematically associated to control volumes K and $L \in \mathcal{T}$ such that $\sigma = K|L$ in summations.

3. Discrete functional analysis

3.1. Discrete gradients.

Definition 3. ***(Discrete gradient).***
We denote by $\nabla^h_{\mathcal{E}}$ the discrete gradient operator mapping scalar fields $U \in \mathbb{C}^{d_h}$ into vector fields of $(\mathbb{C}^2)^{e_h}$ (where we recall that e_h denotes the number of edges in the mesh $\mathcal{T}$), where $\nabla^h_{\mathcal{E}} U = (\nabla^h_{\mathcal{E},\sigma})_{\sigma\in\mathcal{E}}$ is defined by

$$\nabla^h_{\mathcal{E},\sigma} U := \begin{cases} d\dfrac{U_L - U_K}{d_{K|L}}\nu_{K,\sigma} & \text{if } \sigma = K|L \in \mathcal{E}_{\rm int}, \\ -d\dfrac{U_K}{d_{K|L}}\nu_{K,\sigma} & \text{if } \sigma \in \mathcal{E}_{\rm ext}. \end{cases}$$

Note that $\nabla^h_{\mathcal{E}} U$ is considered as a piecewise constant function on the *diamond cells* D_σ for any edge $\sigma \in \mathcal{E}$, which are defined (see Figure 2) as the open quadrangle whose diagonals are the edge σ and the segment $[x_K, x_L]$ for $\sigma = K|L \in \mathcal{E}_{\rm int}$.

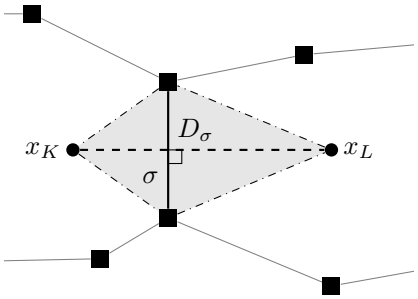

Figure 2. Diamond cell D_σ for $\sigma \in \mathcal{E}_{\rm int}$

We also state the discrete equivalent of the usual integration by parts formula in the context of finite-volume schemes: for U, $\widetilde{U} \in \mathbb{C}^{d_h}$, we have

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K\cap\mathcal{E}_{\rm int}} \frac{|\sigma|}{d_{K|L}}(U_k - U_L)\widetilde{U}_K = \sum_{\sigma\in\mathcal{E}_{\rm int}} \frac{|\sigma|}{d_{K|L}}(U_k - U_L)(\widetilde{U}_K - \widetilde{U}_L)$$

rearranging the sum on the left-hand side.

3.2. Discrete Gagliardo-Nirenberg inequalities.

From classical Sobolev embeddings, we know that $\|f\|_{L^\infty(\Omega)} \le C_{\Omega,\varepsilon}\|f\|_{H^{1+\varepsilon}(\Omega)}$ with $d=2$ or $\|f\|_{L^\infty(\Omega)} \le C_{\Omega,\varepsilon}\|f\|_{H^{\frac{3}{2}+\varepsilon}(\Omega)}$ with $d=3$ for any $\varepsilon > 0$, however these estimates do not hold for $\varepsilon = 0$. However, taking advantage of the discrete structures of the space H^1_h, and relying on inverse estimate for discrete Lebesgue space as well as discrete Sobolev embeddings [5] for L^p_h norms, one can show non-uniform discrete Sobolev embeddings for L^∞_h norm.

Lemma 1. *Let $\Omega \subset \mathbb{R}^d$ be a connected bounded open polygonal or polyhedral set, and $\mathcal{T}$ an admissible finite-volume mesh with mesh size $h > 0$ satisfying the regularity property (reg). Then there exists a constant $C = C_{\Omega,\xi} > 0$ such that*

$$\|U\|_{L^\infty_h} \leq C_{\Omega,\xi} \begin{cases} |\log h| \|U\|_{H^1_h} & \text{if } d = 2, \\ h^{-\frac{1}{2}} \|U\|_{H^1_h} & \text{if } d = 3. \end{cases}$$

Proof. We only sketch the proof for $d = 2$, which can also be found in [8, Corollary 1] for $d = 2, 3$. There exists $K_0 \in \mathcal{T}$ such that $\|U\|_{L^\infty_h} = |U(K_0)|$, so

$$\|U\|_{L^\infty_h} \leq C h^{-\frac{2}{p}} \|U\|_{L^p_h}$$

where $C = C(\xi)$ depends on the regularity of the mesh. From [5], we then have the discrete Gagliardo-Nirenberg inequality

$$\|U\|_{L^p_h} \leq C_{\Omega,\xi} p \|U\|_{H^1_h}.$$

as the constant $C(p)$ depends linearly on $p \geq 1$ in the proof of [5, Theorem 4.3]. We then infer that

$$\|U\|_{L^\infty_h} \leq C h^{-\frac{2}{p}} p \|U\|_{H^1_h}$$

so taking $p = |\log h|$ gives the result. □

Lemma 2. *Let $\Omega \subset \mathbb{R}^d$ be a connected bounded open polygonal or polyhedral set, and $\mathcal{T}$ an admissible finite-volume mesh with mesh size $h > 0$ satisfying the regularity property (reg). Then there exists a constant $C = C_{\Omega,\xi} > 0$ such that*

$$\|UW\|_{H^1_h} \leq C_{\Omega,\xi} \begin{cases} |\log h| \|U\|_{H^1_h} \|W\|_{H^1_h} & \text{if } d = 2, \\ h^{-\frac{1}{2}} \|U\|_{H^1_h} \|W\|_{H^1_h} & \text{if } d = 3. \end{cases}$$

Proof. We write

$$\|UW\|^2_{H^1_h} = \sum_{\sigma \in \mathcal{E}_{\rm int}} \frac{m_\sigma}{d_\sigma} |U_L W_L - U_K W_K|^2 \lesssim \sum_{\sigma \in \mathcal{E}_{\rm int}} \frac{m_\sigma}{d_\sigma} |u_L|^2 |v_L - v_K|^2 + \sum_{\sigma \in \mathcal{E}_{\rm int}} \frac{m_\sigma}{d_\sigma} |W_K|^2 |U_L - U_K|^2$$

so that

$$\|UW\|_{H^1_h} \lesssim \left(\|U\|_{L^\infty_h} \|W\|_{H^1_h} + \|U\|_{H^1_h} \|W\|_{L^\infty_h} \right)$$

and we conclude using Lemma 1. □

We finally state an estimate which will be useful in the analysis of the stability of the nonlinear discrete flow of our splitting method.

Lemma 3. *Let $t \in \mathbb{R}$ and U, $W \in \mathbb{C}^{d_h}$, then there exists a constant $C = C_{d,\xi,\Omega} > 0$ independent of h such that*

$$\begin{aligned} &\|e^{it|U|^2} U - e^{it|W|^2}\|_{H^1_h} \\ &\qquad \leq 1 + C|t| \left(\|\nabla^h_{\mathcal{E}} U\|_{L^\infty_h} \left(\|U\|_{L^\infty_h} + \|W\|_{L^\infty_h} \right) (1 + |t| \|U\|_{L^\infty_h}) + \|W\|^2_{L^\infty_h} \right) \|U - W\|_{H^1_h}. \end{aligned}$$

Proof. Let's first recall that

$$\|e^{it|U|^2} U - e^{it|W|^2} W\|^2_{\dot{H}^1_h} = \sum_{\sigma \in \mathcal{E}_{\rm int}} \frac{|\sigma|}{d_{K|L}} \left| e^{it|U_K|^2} U_K - e^{it|W_K|^2} W_K - e^{it|U_L|^2} U_L + e^{it|W_L|^2} W_L \right|^2.$$

We can write that

$$\begin{aligned}
&\left|e^{it|U_K|^2}U_K - e^{it|W_K|^2}W_K - e^{it|U_L|^2}U_L + e^{it|W_L|^2}W_L\right| \\
&\quad = \left|e^{it|U_L|^2}(U_K - U_L) - e^{it|W_L|^2}(W_K - W_L) + \left(e^{it(|U_L|^2-|U_K|^2)} - 1\right)e^{it|U_K|^2}U_K\right. \\
&\qquad\qquad \left. - \left(e^{it(|W_L|^2-|W_K|^2)} - 1\right)e^{it|W_K|^2}W_K\right| \\
&\quad = \left|(U_K - U_L) - (W_K - W_L) + (U_K - U_L)\left(e^{it(|U_L|^2-|W_L|^2)} - 1\right)\right. \\
&\qquad\qquad \left(e^{it(|U_L|^2-|U_K|^2)} - 1\right)U_K - \left(e^{it(|W_L|^2-|W_K|^2)} - 1\right)W_K \\
&\qquad\qquad \left. + \left(e^{it(|U_L|^2-|U_K|^2)} - 1\right)\left(e^{it(|U_L|^2-|W_L|^2)} - 1\right)U_K\right| \\
&\quad \le |(U_K - U_L) - (W_K - W_L)| + |t||U_K - U_L|\left(|U_L| + |W_L|\right)|U_L - W_L| \\
&\qquad + \underbrace{\left|\left(e^{it(|U_L|^2-|U_K|^2)} - 1\right)U_K - \left(e^{it(|W_L|^2-|W_K|^2)} - 1\right)W_K\right|}_{=:\,\mathcal{A}_{K,L}} \\
&\qquad\qquad + t^2\left(|U_L| + |U_K|\right)|U_L - U_K||U_K|\left(|U_L| + |W_L|\right)|U_L - W_L|,
\end{aligned}$$

and we can bound the third term $\mathcal{A}_{K,L}$ by

$$\begin{aligned}
\mathcal{A}_{K,L} &= \left|\left(e^{it(|U_L|^2-|U_K|^2)} - 1\right)(U_K - W_K) + \left(e^{it(|U_L|^2-|U_K|^2)} - e^{it(|W_L|^2-|W_K|^2)}\right)W_K\right| \\
&\le |t|\left(|U_L| + |U_K|\right)|U_L - U_K||U_K - W_K| + |t|\left||U_L|^2 - |U_K|^2 - |W_K|^2 + |W_L|^2\right||W_K| \\
&\le |t|\left(|U_L| + |U_K|\right)|U_L - U_K||U_K - W_K| + |t||W_K||U_L - U_K|\left(|U_L - W_L| + |U_K - W_K|\right) \\
&\qquad + |t||W_K|\left(|W_L| + |W_K|\right)|U_L - W_L - U_K + W_K|
\end{aligned}$$

after elementary computations and using that $||a| - |b|| \le |a - b|$ for any $a, b \in \mathbb{C}$. In order to get the final estimate, we first remark that for $\sigma = K|L \in \mathcal{E}_{\rm int}$, we have

$$\begin{aligned}
\frac{|\sigma|}{d_{K|L}}|U_K - U_L|^2|W_K - U_K|^2 &= |\sigma|d_{K|L}\left|\frac{U_K - U_L}{d_{K|L}}\right|^2|W_K - U_K|^2 \\
&\le \frac{\|\nabla_{\mathcal{E}}^h U\|_{L_h^\infty}^2}{d^2\xi}|\sigma|d_{K,\sigma}|W_K - U_K|^2 \\
&\le \frac{\|\nabla_{\mathcal{E}}^h U\|_{L_h^\infty}^2}{d^2\xi}\left(|\sigma|d_{K,\sigma}|W_K - U_K|^2 + |\sigma|d_{L,\sigma}|W_L - U_L|^2\right)
\end{aligned}$$

using the regularity assumption of the mesh $\mathcal{T}$, so summing over $\sigma \in \mathcal{E}_{\rm int}$, we infer that

$$\sum_{\sigma\in\mathcal{E}_{\rm int}}\frac{|\sigma|}{d_{K|L}}|U_K - U_L|^2|W_K - U_K|^2 \le \frac{\|\nabla_{\mathcal{E}}^h U\|_{L^\infty}^2}{d^2\xi}\sum_{K\in\mathcal{T}}|K||W_K - U_K|^2.$$

Estimating each term in the given order, we then infer that

$$\begin{aligned}
\|e^{it|U|^2}U - e^{it|W|^2}W\|_{H_h^1} &\le \|U - W\|_{H_h^1} + |t|C_{d,\xi}\|\nabla_{\mathcal{E}}^h U\|_{L_h^\infty}\left(\|U\|_{L_h^\infty} + \|W\|_{L_h^\infty}\right)\|U - W\|_{L_h^2} \\
&\quad + 2|t|\|W\|_{L_h^\infty}^2\|U - W\|_{H_h^1} + 2t^2\|\nabla_{\mathcal{E}}^h U\|_{L_h^\infty}\|U\|_{L_h^\infty}\left(\|U\|_{L_h^\infty} + \|W\|_{L_h^\infty}\right)\|U - W\|_{L_h^2},
\end{aligned}$$

and we get the result using the discrete Poincaré inequality. □

3.3. **Interpolants.** In this section we compare the pointwise interpolant P_h with the mean interpolant π_h defined by

$$(\pi_h\varphi)_K = \varphi_K \coloneqq \frac{1}{|K|}\int_K \varphi(x)\mathrm{d}x$$

for all $K \in \mathcal{T}$ and $\varphi \in L^1(\Omega)$.

Lemma 4. *There exists a constant $C_\xi > 0$ depending only on the regularity ξ of the mesh $\mathcal{T}$ such that for all $\varphi \in H^1(\Omega)$, we have*

$$\|\pi_h\varphi\|_{H_h^1} \leq C_\xi \|\varphi\|_{H^1}.$$

Proof. We recall that

$$\|\pi_h\varphi\|_{H_h^1}^2 = \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} \frac{|\sigma|}{d_{K|L}}|\varphi_K - \varphi_L|^2. \tag{1}$$

For $\sigma \in \mathcal{E}_{\mathrm{int}}$, we denote

$$\varphi_\sigma = \frac{1}{|\sigma|}\int_\sigma \varphi(x)\mathrm{d}\gamma(x).$$

From [9, Lemma B.6.] we infer that there exists $C_\xi > 0$ such that

$$|\varphi_K - \varphi_L|^2 \leq 2\left(|\varphi_K - \varphi_\sigma|^2 + |\varphi_\sigma - \varphi_L|^2\right) \leq \frac{C_\xi}{|\sigma|}\left(h_K\int_K |\nabla\varphi(x)|^2\mathrm{d}x + h_L\int_L |\nabla\varphi(x)|^2\mathrm{d}x\right).$$

Multiplying this inequality by $|\sigma|/d_{K|L}$ and summing over the edges $\sigma \in \mathcal{E}_{\mathrm{int}}$, we get that

$$\sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} \frac{|\sigma|}{d_{K|L}}|\varphi_K - \varphi_L|^2 \leq 2\widetilde{C}_\xi\int_\Omega |\nabla\varphi(x)|^2\mathrm{d}x$$

where $\widetilde{C}_\xi > 0$, recalling that

$$\frac{h_K}{d_{K|L}} = \frac{h_K}{d_{K,\sigma} + d_{L,\sigma}} \leq \frac{h_K}{d_{K,\sigma}} \leq \xi^{-1},$$

which gives the result by Poincaré inequality. □

Lemma 5. *Let $\varphi \in H^3(\Omega)$, then*

$$\|P_h\varphi - \pi_h\varphi\|_{H_h^1} \leq Ch\|\varphi\|_{H^3}.$$

In particular, we infer that

$$\|P_h\varphi\|_{H_h^1} \leq C\left(\|\varphi\|_{H^1} + h\|\varphi\|_{H^3}\right) \leq C\|\varphi\|_{H^3}$$

as soon as $h \leq 1$.

Proof. The second inequality of this lemma is direct in view of Lemma 4, so we focus on the first one. First we write that

$$\|P_h\varphi - \pi_h\varphi\|_{H_h^1}^2 = \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} \frac{|\sigma|}{d_{K|L}}|\varphi(x_K) - \varphi_K - \varphi(x_L) + \varphi_L|^2.$$

For $K \in \mathcal{T}$ and for a.e. $x \in K$, we have by Taylor expansion that

$$\varphi(x) - \varphi(x_K) = \int_0^1 \nabla\varphi(tx_K + (1-t)x)\cdot(x - x_K)\mathrm{d}t.$$

Integrating this expression over $x \in K$ and dividing by $|K|$, we get that

$$\varphi_K - \varphi(x_K) = \frac{1}{|K|}\int_K \int_0^1 \nabla\varphi(tx_K + (1-t)x)\cdot(x - x_K)\mathrm{d}t\mathrm{d}x.$$

As $|x - x_K|^2 \leq h_K^2$, this implies that

$$\frac{|\sigma|}{d_{K,\sigma}}|\varphi_K - \varphi(x_K)|^2 = \frac{|\sigma|}{d_{K,\sigma}}h_K^2 \sup_{y\in K}|\nabla\varphi(y)|^2.$$

We conclude remarking that

$$\frac{|\sigma|}{d_{K|L}}|\varphi(x_K) - \varphi_K - \varphi(x_L) + \varphi_L|^2 \leq 2|\sigma|\left(\frac{|\varphi_K - \varphi(x_K)|^2}{d_{K,\sigma}} + \frac{|\varphi_L - \varphi(x_L)|^2}{d_{L,\sigma}}\right),$$

so summing over $\sigma \in \mathcal{E}_{\mathrm{int}}$ gives that

$$\|P_h\varphi - \pi_h\varphi\|_{H_h^1}^2 \lesssim h^2\|\nabla\varphi\|_{L^\infty}^2 \lesssim h^2\|\varphi\|_{H^3}^2.$$

□

4. The linear case

We first state a useful isometry property concerning the linear flow of the discrete Schrödinger operator with respect to discrete Hilbert Sobolev spaces, which plays a fundamental role in the study of dispersive equations:

Lemma 6. *For all $t \in \mathbb{R}$ and $U \in \mathbb{C}^{d_h}$, we have*

$$\|e^{itA}U\|_{H_h^1} = \|U\|_{H_h^1}.$$

Proof. We denote by $\langle\cdot,\cdot\rangle_{\mathcal{T}}$ the L^2-inner product induced by the mesh $\mathcal{T}$, defined by

$$\langle U, W\rangle_{\mathcal{T}} = \sum_{K\in\mathcal{K}} |K|U_K\overline{W_K}$$

for all U, $W \in \mathbb{C}^{d_h}$. From the definition (2.2) of the discrete laplace operator A and by discrete integration by parts, we have

$$\langle AU, U\rangle_{\mathcal{T}} = \sum_{K\in\mathcal{T}} |K|\overline{U_K}\left(\frac{1}{|K|}\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{E}_{\mathrm{int}}}\frac{|\sigma|}{d_{K|L}}(U_L - U_K)\right) = \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}}\frac{|\sigma|}{d_{K,L}}|U_K - U_L|^2 = \|U\|_{H_h^1}^2.$$

In particular, as A is a real and symmetric matrix with respect to the inner product $\langle\cdot,\cdot\rangle_{\mathcal{T}}$, so e^{itA} is unitary for all $t \in \mathbb{R}$ and we get that

$$\|e^{itA}U\|_{H_h^1} = \langle Ae^{itA}U, e^{itA}U\rangle_{\mathcal{T}} = \langle e^{itA}AU, e^{itA}U\rangle_{\mathcal{T}} = \langle AU, e^{-itA}e^{itA}U\rangle_{\mathcal{T}} = \|U\|_{H_h^1}.$$

□

We now focus on the error performed by the TPFA scheme (2.2) on the semi-discretization of the linear flow on our Voronoï mesh:

Proposition 1. *Let $\varphi \in H^5(\Omega)$ and $t \geq 0$, then*

$$\|P_he^{it\Delta}\varphi - e^{itA}P_h\varphi\|_{H_h^1} \leq Cht\|\varphi\|_{H^5(\Omega)}$$

where $C = C(d, \Omega, \xi) > 0$.

Proof. By the isometry property of Lemma 6 we define ϕ such that

$$\|P_h e^{i\tau\Delta}\varphi - e^{i\tau A}P_h\varphi\|_{H_h^1} = \|\underbrace{e^{-itA}P_h e^{it\Delta}\varphi}_{=:\phi(t)} - \underbrace{P_h\varphi}_{=\phi(0)}\|_{H_h^1},$$

so differentiating with respect to time we get that ϕ satisfies the equation

$$\begin{aligned}\partial_t\phi &= -iA\phi + ie^{-itA}P_h\Delta e^{it\Delta}\varphi\\ &= -iA\phi + ie^{-itA}AP_h\Delta e^{it\Delta}\varphi + ie^{-itA}(P_h\Delta - AP_h)e^{it\Delta}\varphi\\ &= ie^{-itA}(P_h\Delta - AP_h)e^{it\Delta}\varphi\\ &= ie^{-itA}(P_h\Delta - \pi_h\Delta)e^{it\Delta}\varphi + ie^{-itA}(\pi_h\Delta - AP_h)e^{it\Delta}\varphi\end{aligned}$$

Integrating and by isometry, we infer

$$\|\phi(t)-\phi(0)\|_{H_h^1} \le \int_0^t \|(P_h\Delta-\pi_h\Delta)e^{it\Delta}\varphi\|_{H_h^1} + \int_0^\tau \|(\pi_h\Delta - AP_h)e^{i\tau\Delta}\varphi\|_{H_h^1} \tag{2}$$

From Lemma 5 we know that

$$\int_0^t \|(P_h\Delta-\pi_h\Delta)e^{it\Delta}\varphi\|_{H_h^1} \le Ch\|\Delta e^{it\Delta}\varphi\|_{H^3} \le Cht\|\varphi\|_{H^5},$$

We now focus on the estimate for the second term on the right hand side of (2), and we denote by $u = e^{it\Delta}\varphi \in H^5(\Omega)$, so that $\Delta u \in H^3(\Omega) \subset \mathcal{C}(\Omega)$ as $d = 2, 3$. We write that for any $K \in \mathcal{T}_{\rm int}$,

$$(AP_hu - \pi_h\Delta u)_K = \frac{1}{|K|}\sum_{\sigma\in\mathcal{E}_K}|\sigma|\left(\frac{u(x_L)-u(x_K)}{d_{K|L}} - \frac{1}{|\sigma|}\int_\sigma \nabla u\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)\right) = \frac{1}{|K|}\sum_{\sigma\in\mathcal{E}_K}|\sigma|R_{k,\sigma},$$

where $R_{K,\sigma}$ denotes the consistency error of the flux approximation. By Taylor expansions

$$\begin{aligned}u(x_L)-u(x_K) &= (x_L-x_K)\cdot\nabla u(x_K) + \frac{1}{2}(x_L-x_K)\cdot H(x_K)(x_L-x_K)\\ &+ \frac{1}{6}\int_0^1\sum_{j=1}^d\sum_{k=1}^d\sum_{\ell=1}^d \partial_{x_j}\partial_{x_k}\partial_{x_\ell}u(tx_k+(1-t)x_L)(x_{L,j}-x_{K,j})(x_{L,k}-x_{K,k})(x_{L,\ell}-x_{K,\ell})t^2\mathrm{d}t\end{aligned}$$

and

$$\nabla u(x) = \nabla u(x_K) + H(x_K)(x-x_K) + \frac{1}{2}\int_0^1\sum_{j=1}^d\sum_{k=1}^d (x_j-x_{K,j})(x_k-x_{K,k})\partial_{x_j}\partial_{x_k}\nabla u(tx_K+(1-t)x)t\mathrm{d}t,$$

so integrating the last equation on σ and recalling that $\nu_{K,\sigma} = \frac{x_K-x_L}{d_{K|L}}$, we infer

$$\begin{aligned}\int_\sigma \nabla u(x)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x) &= |\sigma|\nabla u(x_K)\cdot\frac{x_L-x_K}{d_{K|L}} + H(x_K)\int_\sigma (x-x_K)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)\\ &+ \frac{1}{2}\int_\sigma\int_0^1\sum_{j=1}^d\sum_{k=1}^d (x_j-x_{K,j})(x_k-x_{K,k})\partial_{x_j}\partial_{x_k}\nabla u(tx_K+(1-t)x)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)t\mathrm{d}t.\end{aligned}$$

As $|x_L-x_k|, |x-x_K| \le 2h$ for all $x\in\sigma$, we have

$$\frac{1}{d_{K|L}}|\partial_{x_j}\partial_{x_k}\partial_{x_\ell}u(tx_k+(1-t)x_L)||x_L-x_K|^3 \le C_\xi h^2\|\partial_{x_j}\partial_{x_k}\partial_{x_\ell}u\|_{L^\infty}$$

and

$$\frac{1}{|\sigma|}\int_\sigma |x-x_K|^2 \left|\partial_{x_j}\partial_{x_k}\nabla u(tx_K+(1-t)x)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)\right| \leq h^2\|\partial_{x_j}\partial_{x_k}\nabla u\|_{L^\infty}$$

for all $1\leq j,k,\ell\leq d$ and $0\leq t\leq 1$ by regularity assumption on the mesh (reg) and as $u\in H^5(\Omega)$, similarly to the proof of [10, Theorem 9.3] we then get that

$$R_{K,\sigma}=\frac{1}{2}\frac{x_L-x_K}{d_{K|L}}\cdot H(x_K)(x_L-x_K)-\frac{1}{|\sigma|}H(x_K)\int_\sigma (x-x_K)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)+\mathcal{O}(h^2).$$

We now decompose our vector $x\in\sigma$ as

$$x=x_K+d_{K,\sigma}\frac{x_L-x_K}{d_{K|L}}+s(x)(x_L-x_K)^\perp$$

where s is a parametrization parameter, which allows to write that

$$\begin{aligned}\int_\sigma (x-x_K)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)&=\frac{d_{K,\sigma}}{d_{K|L}}\int_\sigma (x_L-x_K)\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)+\int_\sigma s(x)(x_L-x_K)^\perp\cdot\nu_{K,\sigma}\mathrm{d}\gamma(x)\\&=\frac{d_{K,\sigma}}{d_{K|L}}(x_L-x_K)\cdot\frac{x_L-x_K}{d_{K|L}}|\sigma|\end{aligned}$$

as we know that the segments $[x_K,x_L]$ and σ are orthogonal. Now we exploit the fact that on Voronoï meshes satisfying assumption (iso), we have $2d_{K,\sigma}=d_{K|L}$ so $R_{K,\sigma}=\mathcal{O}(h^2)$. Note that if $K\in\mathcal{T}_{\mathrm{ext}}$, a similar proof holds taking $u(x_K)=0$ as $x_K\in\partial\Omega$. Summing over $\sigma\in\mathcal{E}_{\mathrm{int}}$, we get that

$$\begin{aligned}\|AP_hu-\pi_h\Delta u\|_{H_h^1}^2&=\sum_{\sigma=K|L}\frac{|\sigma|}{d_{K|L}}\left|\frac{1}{|K|}\sum_{\overline{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_K}|\overline{\sigma}|R_{K,\overline{\sigma}}-\frac{1}{|L|}\sum_{\widetilde{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_L}|\widetilde{\sigma}|R_{K,\widetilde{\sigma}}\right|^2\\&\lesssim\sum_{\sigma=K|L}\frac{|\sigma|}{d_{K|L}}\left(\left|\frac{1}{|K|}\sum_{\overline{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_K}|\overline{\sigma}|R_{K,\overline{\sigma}}\right|^2+\left|\frac{1}{|L|}\sum_{\widetilde{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_L}|\widetilde{\sigma}|R_{K,\widetilde{\sigma}}\right|^2\right)\\&\lesssim\sum_{\sigma=K|L}\frac{|\sigma|}{d_{K|L}}\left(\left|\frac{1}{|K|}\sum_{\overline{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_K}h^{d+1}\right|^2+\left|\frac{1}{|L|}\sum_{\widetilde{\sigma}\in\mathcal{E}_{\mathrm{int}}\cap\mathcal{E}_L}h^{d+1}\right|^2\right)\\&\lesssim\sum_{\sigma=K|L}\frac{|\sigma|}{d_{K|L}}h^2\lesssim Ch^2,\end{aligned}$$

where we have used the fact that there is a uniformly bounded number of edges (or faces) by control volume K, as

$$h_K^d\geq|K|=\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{E}_{\mathrm{int}}}\frac{|\sigma|d_{K,\sigma}}{d}\geq\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{E}_{\mathrm{int}}}\frac{h_K^d}{d\xi^2}=\frac{|\mathcal{E}_K|}{d\xi^2}h_K^d,$$

which ends the proof. □

5. Semi-discretization in time and splitting integration

5.1. **Scheme, notations and first properties.** We now describe the semi-discretization in time of the Gross-Pitaevskii equation using a Lie-Trotter scheme. The analysis of such splitting methods for nonlinear Schrödinger equations are now well understood (in particular we refer to the recent work [23]), and we briefly give its proof here mainly for clearness and completeness purposes.

The operator splitting methods for the time integration of equation (GP) are based on the following splitting

$$\partial_t \psi = A(\psi) + B(\psi),$$

where

$$A(\psi) = i\Delta\psi, \quad B(\psi) = -i|\psi|^2\psi - iV\psi,$$

and the solutions of the subproblems

$$\begin{cases} i\partial_t v(t,x) = -\Delta v(t,x), & v(0,x) = v_0(x), \\ i\partial_t w(t,x) = |w(t,x)|^2 w(t,x) + V(t,x)w(t,x), & w(0,x) = w_0(x), \end{cases}$$

for all $x \in \Omega$ and $t > 0$. The associated operators are explicitly given for $t > 0$ by the flows

$$v(\tau) = \Phi_A^\tau(v_0) := e^{i\tau\Delta} v_0$$

and

$$w(\tau) = \Phi_B^{t,\tau}(w_0) := e^{-i\int_0^\tau V(t+s)\mathrm{d}s - i\tau|w_0|^2} w_0.$$

We denote by $u^0 = \psi_0$ the initial state. The *Lie-Trotter splitting* scheme then recursively reads as

$$u^n = \Phi^{t_{n-1},\tau}(u^{n-1}), \quad n \geq 1, \quad \Phi^{t,\tau} := \Phi_A^\tau \circ \Phi_B^{t,\tau} \tag{LTSP}$$

for $t \geq 0$. The analysis of such splitting method relies on two main ingredients. We will extensively use the algebra property of Sobolev spaces in dimension $d = 2$ or 3, namely

$$\|fg\|_{H^3} \leq C_d \|f\|_{H^3} \|g\|_{H^3}$$

where $C_d = C(d,\Omega) > 0$, as well as other classical Sobolev estimates for products. We also emphasize that the flows Φ_A^τ and $\Phi_B^{t,\tau}$ enjoy the following isometric properties: for all $k \in \mathbb{N}$,

$$\|\Phi_A^t(u)\|_{H^k} = \|u\|_{H^k} \quad \text{and} \quad \|\Phi_B^{t,\tau}(u)\|_{L^2} = \|u\|_{L^2}$$

for any $t \geq 0$. It then naturally follows that the (LTSP) scheme preserves the L^2-norm of the initial state, namely for all $t \geq 0$,

$$\|u^n\|_{L^2} = \|\Phi^{t_{n-1},\tau}(u^{n-1})\|_{L^2} = \|u^{n-1}\|_{L^2} = \cdots = \|u^0\|_{L^2} = \|\psi_0\|_{L^2},$$

which makes it particularly appealing from the numerical point of view.

5.2. **Error estimate.** We denote by

$$B_{m_3} = \left\{ v \in H^3(\Omega) \;\middle|\; \|v\|_{H^3} \leq m_3 \right\}$$

the ball of radius $m_3 = \|\psi\|_{L^\infty_T H^3}$. We rely on two properties of the flow $\Phi^{t,\tau}$ in order to show its first order convergence, the *stability property* and the *local error* in $H^3(\Omega)$, that we now state and prove:

Lemma 7. ***(Stability).***
Let $f, g \in B_{m_3}$ and $0 \leq t \leq T - \tau$, then

$$\|\Phi^{t,\tau} f - \Phi^{t,\tau} g\|_{H^3} \leq e^{M\tau} \|f - g\|_{H^3}$$

where $M = M(d, m_3, \|V\|_{L^\infty_T H^3}) > 0$.

Proof. Let's first note that for any $u \in H^3(\Omega)$, we have $\nabla(e^{-i\tau|u|^2}) = -2i\tau \operatorname{Re}(\overline{u}\nabla u)e^{-i\tau|u|^2}$,

$$\Delta(e^{-i\tau|u|^2}) = -2i\tau\left(\nabla u\cdot\nabla u + \overline{u}\Delta u - 2i\tau \operatorname{Re}(\overline{u}\nabla u)\cdot\operatorname{Re}(\overline{u}\nabla u)\right)e^{-i\tau|u|^2},$$

and

$$\begin{aligned}\nabla\Delta(e^{-i\tau|u|^2}) = -2i\tau\big(&\nabla(\nabla u\cdot\nabla u) + \overline{u}\nabla\Delta u + \nabla\overline{u}\Delta u - 2i\tau\nabla(\operatorname{Re}(\overline{u}\nabla u)\cdot\operatorname{Re}(\overline{u}\nabla u))\\ &-2i\tau\operatorname{Re}(\overline{u}\nabla u)\left(\nabla u\cdot\nabla u + \overline{u}\Delta u - 2i\tau\operatorname{Re}(\overline{u}\nabla u)\cdot\operatorname{Re}(\overline{u}\nabla u)\right)\big)e^{-i\tau|u|^2}\end{aligned}$$

so taking L^2-norms of the above expressions, we infer by Hölder's inequality and Sobolev embedding $H^1(\Omega)\subset L^6(\Omega)$ and $H^2(\Omega)\subset L^\infty(\Omega)$ that

$$\|e^{-i\tau|u|^2}\|_{H^3} \le C(1+\|u\|_{H^3}^6).$$

The same way, we get that

$$\|e^{-i\int_0^\tau V(t+s)\mathrm{d}s}\|_{H^3} \le C(1+\|V\|^2_{L^\infty_T H^3}),$$

so taking now $u\in B_{m_3}$, we have

$$\|\Phi_B^{t,\tau}u\|_{H^3} \le C_d^2\|e^{-i\int_0^\tau V(t+s)\mathrm{d}s}\|_{H^3}\|e^{-i\tau|u|^2}\|_{H^3}\|u\|_{H^3} \le M_0\|u\|_{H^3}$$

where $M_0 = M_0(d,t,m_3,\|V\|_{L^\infty_T H^3})>0$. By Duhamel's formula, we can write that

$$\Phi_B^{t,\tau}f = f + \int_0^\tau V(t+s)\Phi_B^{s,\tau}f(s)\mathrm{d}s + \int_0^\tau |\Phi_B^{s,\tau}f(s)|^2\Phi_B^{s,\tau}f(s)\mathrm{d}s,$$

and the same formula holds for $\Phi_B^{t,\tau}g$, so applying Φ_A^τ and by isometry we infer

$$\begin{aligned}\|\Phi^{t,\tau}f - \Phi^{t,\tau}g\|_{H^3} \le \|f-g\|_{H^3} &+ C_d\|V\|_{L^\infty_T H^3}\int_0^\tau \|\Phi^{t,s}f - \Phi^{t,s}g\|_{H^3}\mathrm{d}s\\ &+ \frac{3}{2}C_d^2\underbrace{\left(\|\Phi^{t,\tau}f\|^2_{H^3} + \|\Phi^{t,\tau}g\|^2_{H^3}\right)}_{\le 2M_0^2m_3^2}\int_0^\tau \|\Phi^{t,s}f - \Phi^{t,s}g\|_{H^3}\mathrm{d}s\end{aligned}$$

and we get the result by Gronwall lemma. □

Lemma 8. ***(Local error).***
For any $0\le n<N$, we have

$$\|\psi(t_{n+1}) - \Phi^{t,\tau}(\psi(t_n))\|_{H^3} \le C\tau^2,$$

where $C = C(d,m_5,\|V\|_{L^\infty_T H^5})>0$.

Proof. The idea is to compare Taylor expansions in Duhamel's formula

$$\begin{aligned}
\psi(t_{n+1}) &= e^{i\tau\Delta}\psi(t_n) - i\int_0^\tau e^{i(\tau-s)\Delta}\left(V(t_n+s)+|\psi(t_n+s)|^2\right)\psi(t_n+s)\mathrm{d}s \\
&= e^{i\tau\Delta}\psi(t_n) - ie^{i\tau\Delta}\left(\int_0^\tau V(t_n+s)\mathrm{d}s\right)\psi(t_n) - i\tau e^{i\tau\Delta}|\psi(t_n)|^2\psi(t_n) \\
&\quad - e^{i\tau\Delta}\int_0^\tau \underbrace{\int_0^1 e^{-is\theta}(s\Delta)\left(V(t_n+s)+|\psi(t_n+s)|^2\right)\psi(t_n+s)\mathrm{d}\theta}_{=:\mathcal{I}_1(s)}\,\mathrm{d}s \\
&\quad - ie^{i\tau\Delta}\int_0^\tau \underbrace{\left[V(t_n+s)(\psi(t_n+s)-\psi(t_n)) + |\psi(t_n+s)|^2\psi(t_n+s) - |\psi(t_n)|^2\psi(t_n)\right]}_{=:\mathcal{I}_2(s)}\mathrm{d}s
\end{aligned}$$

and

$$\begin{aligned}
\Phi^{t,\tau}(\psi(t_n)) &= e^{i\tau\Delta}e^{-i\int_0^\tau V(t_n+s)\mathrm{d}s - i\tau|\psi(t_n)|^2}\psi(t_n) \\
&= e^{i\tau\Delta}\psi(t_n) - ie^{i\tau\Delta}\left(\int_0^\tau V(t_n+s)\mathrm{d}s\right)\psi(t_n) - i\tau e^{i\tau\Delta}|\psi(t_n)|^2\psi(t_n) \\
&\quad - e^{i\tau\Delta}\underbrace{\int_0^1 (1-\theta)e^{-i\theta(\int_0^\tau V(t_n+s)\mathrm{d}s+\tau|\psi(t_n)|^2)}\mathrm{d}\theta\left(\int_0^\tau V(t_n+s)\mathrm{d}s+\tau|\psi(t_n)|^2\right)^2\psi(t_n)}_{=:\mathcal{I}_3}
\end{aligned}$$

so that

$$\|\psi(t_{n+1}) - \Phi^{t,\tau}(\psi(t_n))\|_{H^3} \le \int_0^\tau \left(\|\mathcal{I}_1(s)\|_{H^3} + \|\mathcal{I}_2(s)\|_{H^3}\right)\mathrm{d}s + \mathcal{I}_3$$

by isometry. Using Sobolev estimates we readily bound the first term

$$\int_0^\tau \|\mathcal{I}_1(s)\|_{H^3}\mathrm{d}s \le \tau^2 C_d^3\left(\|V\|_{L^\infty_T H^5} + m_5^3\right)$$

as well as the third term

$$\|\mathcal{I}_3\|_{H^3} \le \tau^2 C_d^3 m_3\left(\|V\|^2_{L^\infty_T H^3} + m_3^4\right)\sup_{0\le\theta\le1}\left\|e^{-i\theta(\int_0^\tau V(t_n+s)+\tau|\psi(t_n)|^2)}\right\|_{H^3}$$

recalling from the proof of Lemma 7 that

$$\left\|e^{-i\theta(\int_0^\tau V(t_n+s)+\tau|\psi(t_n)|^2)}\right\|_{H^3} \le C(d, m_3, \|V\|_{L^\infty_T H^3})$$

as $0 \le \theta \le 1$. Finally,

$$\begin{aligned}
\int_0^\tau \|\mathcal{I}_2(s)\|_{H^3}\mathrm{d}s &\le C_d\left(\|V\|_{L^\infty_T H^3} + m_2^2\right)\int_0^\tau \|\psi(t_n+s)-\psi(t_n)\|_{H^3}\mathrm{d}s \\
&\le \tau^2 C(d, m_3, \|V\|_{L^\infty_T H^3})\|\partial_t\psi\|_{L^\infty_T H^3},
\end{aligned}$$

so we just need to show that $\|\partial_t\psi\|_{L^\infty_T H^3} < \infty$. In fact, we directly read from equation (GP) that

$$\|\partial_t\psi\|_{L^\infty_T H^3} \le \|\Delta\psi\|_{L^\infty_T H^3} + \||\psi|^2\psi\|_{L^\infty_T H^3} + \|V\psi\|_{L^\infty_T H^3} \le m_4 + C_d^2 m_3^3 + C_d m_3\|V\|_{L^\infty_T H^3},$$

which ends the proof. □

We now give the main result of this section, which states the first order time convergence of the (LTSP) scheme:

Proposition 2. *Let $\psi_0 \in H^5(\Omega)$. We denote by ψ the solution of equation (GP) with initial data $\psi(0) = \psi_0$, and by $(u^n)_{0\leq n\leq N}$ the numerical solution defined by the Lie-Trotter splitting scheme (LTSP) with initial data $u^0 = \psi_0$. Then, there exists $\tau_0 > 0$ such that for all $0 < \tau \leq \tau_0$ and all $0 \leq n \leq N$,*

$$\|\psi(t_n) - u^n\|_{H^3} \leq C\tau,$$

where $C = C(d, m_5, \|V\|_{L^\infty_T H^5})$ is independent of $N = T/\tau$.

Proof. We will prove by induction that the numerical solution $(u^n)_{0\leq n\leq N}$ is uniformly bounded in $H^3(\Omega)$, which will induce the convergence result. More precisely, we will show that for all $0 \leq n \leq N$, $u^n \in B_{m_3+1}$. The case $n = 0$ stands as $u^0 = \psi_0$. We now assume that $u^k \in B_{m_3+1}$ for all $0 \leq k \leq n < T/\tau$, so we need to prove the result on u^{n+1}. Using both Lemma 7 and Lemma 8, we infer that

$$\begin{aligned}\|\psi(t_{n+1}) - u^{n+1}\|_{H^3} &\leq \|\psi(t_{n+1}) - \Phi^{t,\tau}(\psi(t_n))\|_{H^3} + \|\Phi^{t,\tau}(\psi(t_n)) - \Phi^{t,\tau}(u^n)\|_{H^3} \\ &\leq C\tau^2 + e^{M\tau}\|\psi(t_n) - u^n\|_{H^3} \\ &\leq C\tau^2 \sum_{k=0}^{n} e^{Mk\tau}\end{aligned}$$

where the last inequality is obtained by a recursive procedure. As a sum of terms of a geometric sequence we get that

$$\|\psi(t_{n+1}) - u^{n+1}\|_{H^3} \leq C\tau \frac{e^{MT} - 1}{M}, \tag{3}$$

so for $0 < \tau \leq \tau_0 \coloneqq \frac{M}{C(e^{MT}-1)}$ we have that

$$\|u^{n+1}\|_{H^3} \leq \|\psi(t_{n+1})\|_{H^3} + 1 \leq m_3 + 1$$

so $u^{n+1} \in B_{m_3+1}$, which ends the induction proof. The convergence result then follows from equation (3). □

5.3. **Boundedness of higher Sobolev norms.** We end up this section with a last property which will be useful afterwards, stating that the semi-discrete numerical solution $(u^n)_{0\leq n\leq N}$ is in fact uniformly bounded in $H^5(\Omega)$.

Lemma 9. *Let $0 < \tau \leq \tau_0$ and $M_2 > 0$ independent of N and τ such that*

$$\sup_{0\leq n\leq N} \|u^n\|_{H^2} \leq M_2.$$

Then there exists $M_5 > 0$ independent of N and τ such that

$$\sup_n \|u^n\|_{H^5} \leq M_5.$$

Proof. We note that $\Phi_B^{t,\tau}\varphi$ is solution of the ODE

$$i\dot{\eta} = |\varphi|^2\eta + V(t)\eta, \quad \eta(0) = \varphi,$$

so by Sobolev estimates we get that

$$\|\dot{\eta}(t)\|_{H^5} \lesssim \|\varphi\|^2_{H^2}\|\eta(t)\|_{H^5} + \|\varphi\|_{H^2}\|\eta(t)\|_{H^2}\|\varphi\|_{H^5} + \|V(t)\|_{H^5}\|\eta(t)\|_{H^5}.$$

Integrating in time and recalling that $u^{n+1} = \Phi^{t_n,\tau}(u^n)$ we infer that

$$\|\Phi^{t_n,\tau}(u^n)\|_{H^5} \leq \|u^n\|_{H^5}(1 + \tau M_2^2) + (2M_2^2 + \|V\|_{L^\infty_T H^2}) \int_{t_n}^{t_{n+1}} \|\Phi^{s,\tau}(u^n)\|_{H^5} \mathrm{d}s$$

by isometry, so from Gronwall lemma we get that

$$\|u^{n+1}\|_{H^5} \leq (1+M_2^2\tau)e^{\tau\left(2M_2^2+\|V\|_{L^\infty_T H^5}\right)}\|u^n\|_{H^5},$$

which in turns recursively gives that

$$\|u^n\|_{H^5} \leq e^{T\left(3M_2^2+\|V\|_{L^\infty_T H^5}\right)}\|u^0\|_{H^5}$$

for all $0 \leq n \leq N$, which gives the result as $u^0 = \psi_0$. □

6. Convergence of the fully discrete scheme

Having now all the tools at hand, we turn to the proof of Theorem 1. First of all we write for $0 \leq n < T/\tau$ that

$$\|P_h(\psi(t_{n+1})) - U^{n+1}\|_{H^1_h} \leq \|P_h(\psi(t_{n+1})) - P_h(u^{n+1})\|_{H^1_h} + \|P_h(u^{n+1}) - U^{n+1}\|_{H^1_h}.$$

From Lemma 5 and Proposition 2 we can easily bound the first term by

$$\|P_h(\psi(t_{n+1})) - P_h(u^{n+1})\|_{H^1_h} \leq C_\xi \|\psi(t_{n+1}) - u^{n+1}\|_{H^3} \leq C\tau,$$

where $C = C(\xi, d, m_5, \|V\|_{L^\infty_T H^5})$. For the other term, by isometry and definition of U^{n+1} we have

$$\begin{aligned}\|P_h(u^{n+1}) - U^{n+1}\|_{H^1_h} \leq{}& \|P_h e^{i\tau\Delta}u^n - e^{i\tau A}P_h u^n\|_{H^1_h} \\ &+ \|P_h(e^{-iG_n(\tau)-i\tau|u^n|^2}u^{n-1}) - e^{-iP_hG_n(\tau)}P_h(e^{-i\tau|u^n|^2}u^n)\|_{H^1_h} \\ &+ \|e^{-iP_hG_n(\tau)}\left(P_h(e^{-i\tau|u^n|^2}u^n) - e^{-i\tau|U^n|^2}U^n\right)\|_{H^1_h}.\end{aligned}$$

As the pointwise interpolant P_h satisfies $P_h(fg) = P_h(f)P_h(g)$ for any $f, g \in \mathcal{C}(\Omega)$ (and so $P_h e^f = e^{P_h f}$), by regularity of V and u^n the second term in the above estimate vanishes. A direct bound on the first term comes as a consequence of Proposition 1, so that

$$\|P_h e^{i\tau\Delta}u^n - e^{i\tau A}P_h u^n\|_{H^1_h} \leq Ch\tau,$$

where $C = C(m_5, d, \xi, M_5) > 0$. Finally, by discrete Sobolev inequality Lemma 2 and stability of the interpolant P_h Lemma 5 we get that

$$\|e^{-iP_hG_n(\tau)}\left(e^{-i\tau|P_hu^n|^2}P_hu^n - e^{-i\tau|U^n|^2}U^n\right)\|_{H^1_h} \leq C|\log h|\tau\|P_h(e^{-i\tau|u^n|^2}u^n) - e^{-i\tau|U^n|^2}U^n\|_{H^1_h}$$

where $C = C(d, \xi, \|V\|_{L^\infty_T H^4})$ in the case $d = 2$ (the same hold in dimension $d = 3$ with $h^{-\frac{1}{2}}$ instead of $|\log h|$ in the previous estimate). From the CFL condition $\sqrt{\tau}|\log h| \leq 1$ if $d = 2$ or $\tau \leq h$ if $d = 3$, we infer the existence of a $\tilde{\tau}_0 > 0$ independent of τ and h such that $C|\log h|\tau \leq 1$ or $Ch^{-\frac{1}{2}}h \leq 1$, so gathering the bounds we have

$$\|P_h(u^{n+1}) - U^{n+1}\|_{H^1_h} \leq Ch\tau + \|e^{-i\tau|P_hu^n|^2}P_hu^n - e^{-i\tau|U^n|^2}U^n\|_{H^1_h}. \tag{4}$$

In the same vein of the proof of Proposition 2, we will now prove that the numerical solution $(U^n)_n$ is uniformly bounded in L^∞_h. We recall that $M_5 \coloneqq \sup_{0\leq n\leq N}\|u^n\|_{H^5(\Omega)}$ is independent of N in view of Lemma 9, and we define

$$B^h_R = \left\{U \in L^\infty_h(\Omega) \;\middle|\; \|U\|_{L^\infty_h} \leq R\right\}$$

be the ball of radius R in $L^\infty_h(\Omega)$ with $R = C_d M_5$, where $C_d > 0$ denotes the constant appearing in the continuous Sobolev embedding

$$\|u\|_{L^\infty} \leq C_d\|u\|_{H^5}.$$

We will show by induction that for all $0 \leq n \leq N$, $U^n \in B^h_{R+1}$. The case $n = 0$ is direct from properties of P_h and Sobolev embedding, namely

$$\|U^0\|_{L^\infty_h} \leq \|P_h u^0\|_{L^\infty_h} \leq \|\psi_0\|_{L^\infty} \leq C_d \|\psi_0\|_{H^2} \leq R.$$

We now assume that $U^n \in B^h_{R+1}$ for all $0 \leq k \leq n$. Going back to estimate (4), in view of Lemma 3 taking $U = P_h u^n$ and $W = U^n$, we write that

$$\begin{aligned}\|P_h u^{n+1} - U^{n+1}\|_{H^1_h} &\leq Ch\tau + \|e^{-i\tau|P_h u^n|^2} P_h u^n - e^{-i\tau|U^n|^2} U^n\|_{H^1_h} \\ &\leq Ch\tau + (1 + C_{d,\xi,\Omega}\tau(M_5^2 + R^2))\|P_h u^n - U^n\|_{H^1_h}\end{aligned}$$

as $\|\nabla^h_{\mathcal{E}} P_h u^n\|_{L^\infty_h} \leq d\|\nabla u^n\|_{L^\infty} \leq CM_5$, so by a recursive argument as in the proof of Proposition 2 we infer that

$$\|P_h u^{n+1} - U^{n+1}\|_{H^1_h} \leq Ch \frac{e^{C_{d,\xi,\Omega} T(M_5^2+R^2)} - 1}{C_{d,\xi,\Omega}(M_5^2 + R^2)} \tag{5}$$

as $U^0 = P_h u^0$. In view of equation (5), we now compute (for the case $d = 2$) that

$$\begin{aligned}\|U^{n+1}\|_{L^\infty_h} &\leq \|P_h u^{n+1}\|_{L^\infty_h} + \|P_h u^{n+1} - U^{n+1}\|_{L^\infty_h} \\ &\leq \|u^{n+1}\|_{L^\infty} + C_d|\log h|\|P_h u^{n+1} - U^{n+1}\|_{H^1_h} \\ &\leq R + C_d|\log h|h \frac{e^{C_{d,\xi,\Omega} T(M_4^2+R^2)} - 1}{C_{d,\xi,\Omega}(M_4^2 + R^2)},\end{aligned}$$

so as $|\log h|h \to 0$ as $h \to 0$, for $0 < h \leq h_0$ small enough we have

$$\|U^{n+1}\|_{L^\infty_h} \leq R + 1$$

and the induction proof is completed (the same holds in dimension 3 as $h^{-\frac{1}{2}} h \to 0$ as $h \to 0$). In particular, R is independent of τ and h, and we infer the first order convergence of $P_h u^{n+1} - U^{n+1}$ in H^1_h-norm from equation (5), which ends the proof.

7. Pseudo-vorticity

In quantum fluid mechanics, the vorticity of the fluid is equal to an identically zero field except at the vortex points where it corresponds to a Dirac δ-function, making it difficult to use in order to numerically identify vortices. On the other hand, the pseudo-vorticity field of the wave function ψ constitutes a very accurate, efficient and robust numerical method to track vortex points in 2D or vortex lines in 3D [22, 25]. This quantity can be defined as $\omega(\psi) = \frac{1}{2}\nabla \times J$, where $J = \mathrm{Im}\left(\overline{\psi}\nabla\psi\right)$ denotes the density current of the quantum fluid. A simple calculation shows that the pseudo-vorticity can be expressed as

$$\omega(\psi) = \frac{1}{4i}\left(\nabla\overline{\psi} \times \nabla\psi - \nabla\psi \times \nabla\overline{\psi}\right) = \nabla\left(\frac{\psi + \overline{\psi}}{2}\right) \times \nabla\left(\frac{\psi - \overline{\psi}}{2i}\right) = \mathrm{Re}\,\nabla\psi \times \mathrm{Im}\,\nabla\psi,$$

where the latter expression has the numerical advantage of only requiring the computation of one derivative of the wave function ψ. Also note that for a regular ψ, the pseudo-vorticity field ω remains regular even at the axis of the vortices. One can also remark that the pseudo-vorticity corresponds to a finite positive or negative field at the vortex core, depending on the winding number ± 1 of the vortex, and vanishes outside.

In order to reconstruct a discrete gradient $\nabla_{\mathcal{T}}^h$ of a vector $U \in \mathbb{C}^{d_h}$ on each control volume $K \in \mathcal{T}$, following [11, Definition 2.3] we define

$$(\nabla_{\mathcal{T}}^h U)_K = \frac{1}{|K|} \sum_{\sigma \in \mathcal{E}_{\rm int} \cap \mathcal{E}_K} \frac{|\sigma|}{d_{K|L}} (U_L - U_K)(x_\sigma - x_K),$$

where x_σ denotes the intersection point between the line (x_K, x_L) and the edge σ. We now state a property showing that our numerical scheme can also be used to accurately compute the pseudo-vorticity field:

Proposition 3. *We assume that ψ and $(U^n)_{0\leq n\leq N}$ are given by Theorem 1. We denote by*

$$\omega_h(U^n) = \operatorname{Re} \nabla_{\mathcal{T}}^h U^n \times \operatorname{Im} \nabla_{\mathcal{T}}^h U^n,$$

then

$$\|P_h \omega(\psi(t_n)) - \omega_h(U^n)\|_{L_h^1} \leq C(\tau + h).$$

Proof. First of all, we emphasize that for $\psi(t) \in H^5(\Omega)$, $\omega(\psi) \in W^{1,4}(\Omega)$ which is continuous by Sobolev embeddings, so $P_h\omega(\psi(t_n))$ is well defined. We focus on the two-dimensional case, as the three-dimensional case can be proven analogously. For $d = 2$, the field $\omega(\psi)$ corresponds to a scalar, and we will decompose our analysis between the semi-discrete error and the full-discrete error, namely

$$\|P_h \omega(\psi(t_n)) - \omega_h(U^n)\|_{L_h^1} = \|P_h \left(\omega(\psi(t_n)) - \omega(u^n)\right)\|_{L_h^1} + \|P_h(\omega(u^n)) - \omega_h(U^n)\|_{L_h^1}. \tag{6}$$

To estimate the first term, we get by Taylor expansion that

$$\|P_h\varphi - \pi_h\varphi\|_{L_h^1} \leq Ch\|\varphi\|_{W^{1,1}(\Omega)}$$

for any $\varphi \in W^{1,1}(\Omega)$, and that

$$\|\pi_h\varphi\|_{L_h^1} = \sum_{K\in\mathcal{T}} |K|(\pi_h\varphi)_K = \sum_{K\in\mathcal{T}} \int_K |\varphi(x)|\mathrm{d}x = \|\varphi\|_{L^1},$$

so we infer

$$\|P_h \left(\omega(\psi(t_n)) - \omega(u^n)\right)\|_{L_h^1} \leq Ch \left(\|\omega(\psi(t_n))\|_{W^{1,1}(\Omega)} + \|\omega(u^n)\|_{W^{1,1}(\Omega)}\right) + \|\omega(\psi(t_n)) - \omega_h^n\|_{L^1}.$$

As $\psi \in \mathcal{C}([0,T], H^5(\Omega))$ and from the Sobolev embbeding $H^2(\Omega) \subset W^{1,1}(\omega)$ (as Ω is bounded), we get that $\|\omega(\psi(t_n))\|_{W^{1,1}(\Omega)}$ and $\|\omega(u^n)\|_{W^{1,1}(\Omega)}$ are uniformly bounded with respect to τ thanks to Lemma 9. On the other hand, writing that

$$\omega(\psi(t_n)) - \omega(u^n) = \operatorname{Re}\nabla\psi(t_n) \times (\operatorname{Im}\nabla\psi(t_n) - \operatorname{Im}\nabla u^n) + (\operatorname{Re}\nabla\psi(t_n) \times \operatorname{Re}\nabla u^n) \times \operatorname{Im}\nabla u^n,$$

by Cauchy-Schwarz we have

$$\|\omega(\psi(t_n)) - \omega_h^n\|_{L^1} \leq \left(\|\nabla\psi(t_n)\|_{L^2} + \|\nabla u^n\|_{L^2}\right) \|\nabla\psi(t_n) - \nabla u^n\|_{L^2}$$

so gathering these bounds and thanks to Proposition 2, we get that

$$\|P_h \left(\omega(\psi(t_n)) - \omega(u^n)\right)\|_{L_h^1} \leq C(h + \tau).$$

We now bound the second term in the right hand side of equation (6). As $P_h\omega(u^n) = P_h(\nabla \operatorname{Re} u^n) \times P_h(\nabla \operatorname{Im} u^n)$, we again get by Cauchy-Schwarz that

$$\|P_h(\omega(u^n)) - \omega_h(U^n)\|_{L_h^1} \leq \left(\|P_h\nabla u^n\|_{L_h^2} + \|\nabla_{\mathcal{T}}^h U^n\|_{L_h^2}\right) \|P_h\nabla u^n - \nabla_{\mathcal{T}}^h U^n\|_{L_h^2}. \tag{7}$$

We directly infer

$$\|\pi_h\varphi\|_{L^2_h}^2 = \sum_{K\in\mathcal{T}} |K| \left(\frac{1}{|K|}\int_K \varphi(x)\mathrm{d}x\right)^2 \leq \sum_{K\in\mathcal{T}} \int_K |\varphi(x)|^2\mathrm{d}x = \|\varphi\|_{L^2}$$

by Jensen inequality, and $\|(P_h - \pi_h)\varphi\|_{L^2_h} \leq Ch\|\varphi\|_{H^3}$ by Taylor expansion, so $\|P_h\nabla u^n\|_{L^2_h}$ is uniformly bounded with respect to τ and h. On the other hand, from [11, Lemma 2.2] we know that

$$\|\nabla^h_{\mathcal{T}} U^n\|_{L^2_h} \leq C_\xi \|U^n\|_{H^1_h} \lesssim \|P_h u^n\|_{H^1_h} + \|P_h u^n - U^n\|_{H^1_h} \leq C(1+h)$$

applying Theorem 1. We then bound the remaining term of equation (7) using the results from Section 6, so

$$\|P_h\nabla u^n - \nabla^h_{\mathcal{T}} U^n\|_{L^2_h} \leq \|P_h\nabla u^n - \nabla^h_{\mathcal{T}} P_h u^n\|_{L^2_h} + \underbrace{\|\nabla^h_{\mathcal{T}} P_h u^n - \nabla^h_{\mathcal{T}} U^n\|_{L^2_h}}_{\leq C_\xi \|P_h u^n - U^n\|_{H^1_h} \leq Ch}.$$

In order to estimate the strong convergence of the discrete gradient $\nabla^h_{\mathcal{T}} P_h u^n$ towards the pointwise interpolant of the gradient $P_h\nabla u^n$, we rely on [11, Lemma 2.5] which states that

$$\|\pi_h\nabla u^n - \nabla^h_{\mathcal{T}} P_h u^n\|_{L^2_h} \leq C_{\xi,\Omega} h \|u^n\|_{H^4},$$

so we write that

$$\|P_h\nabla u^n - \nabla^h_{\mathcal{T}} P_h u^n\|_{L^2_h} \leq \underbrace{\|P_h\nabla u^n - \pi_h\nabla u^n\|_{L^2_h}}_{\leq Ch\|u\|_{H^3}} + \|\pi_h\nabla u^n - \nabla^h_{\mathcal{T}} P_h u^n\|_{L^2_h},$$

which ends the proof. □

8. Numerical simulations

In this section, we report numerical results in dimension $d = 2$ of the proposed numerical method. We take Ω as a polygonal approximation of the open disk $\mathcal{D}(0,2)$ of center $(0,0) \in \mathbb{R}^2$ and of radius 2. To generate an admissible finite volume mesh, we use the GMSH software [15] with the "Frontal-Delaunay" option. Although not stricly giving a Voronoï mesh, this procedure provides a Delaunay triangulation with equilateral triangles on most of the inner part of the disk (which locally stands as a Voronoï mesh), and acute triangles on the boundary. This triangulation is composed of $d_h = 57048$ triangles with a stepsize control parameter $h = 0.04$.

The initial condition is taken as a radial centered Gaussian $\psi_0(x) = e^{-2|x|^2}$, and the time-dependent potential is an harmonic trap of size V_0 perturbed by a rotating sinusoidal stirrer of size ε and frequency ω, which writes

$$V(t,x) = V_0 r^2 \left(1 + \varepsilon\cos(2\theta - \omega t)\right), \quad x = (r,\theta),$$

in polar coordinates. In the upcoming simulations we will take $V_0 = 100$ and $\varepsilon = 0.2$. We also put a positive constant $\lambda = 100$ in front of the cubic nonlinearity $|\psi|^2\psi$ in equation (GP) in order to enhance vortex nucleation. The linear flow Φ^τ_A is computed using a two-order Padé approximant

$$e^{i\tau A} \simeq \left(\mathrm{Id}_{d_h} - i\frac{\tau}{2}A\right)^{-1}\left(\mathrm{Id}_{d_h} + i\frac{\tau}{2}A\right)$$

which also preserves the L^2-norm of the numerical solution. We emphasize that the matrix A is a sparse matrix, so that the resolution of the linear system $AX = B$ can be efficiently precomputed using its sparse LU decomposition. All codes are available on the Gitlab page https://plmlab.math.cnrs.fr/chauleur/codes/-/tree/main/FVGP_codes.

8.1. **Accuracy test.** Let $\Delta t > 0$. We denote by $U^T_{\Delta t}$, $U^T_{2\Delta t}$ and $U^T_{\frac{\Delta t}{2}}$ the numerical solutions obtained at time $t = T$ with the scheme (LT) applied to initial condition $U^0 = P_h\psi_0$ with respectively $\tau = \Delta t$, $\tau = 2\Delta t$ and $\tau = \frac{\Delta t}{2}$. A classical estimate for the time order m_{LT} of the scheme (LT) is then given by the extrapolation formula

$$m_{\mathrm{LT}} = \log\left(\frac{\|U_{2\Delta t} - U_{\Delta t}\|_{H^1_h}}{\|U_{\Delta t} - U_{\frac{\Delta t}{2}}\|_{H^1_h}}\right)\log(2)^{-1} + \mathcal{O}\left(\Delta t\right).$$

We perform several simulations of (GP) with $T = 0.1$, $\omega = 1$ and $N = 2^k$ time discretization points for varying $k \in \mathbb{N}^*$, which we report in the following table, corroborating the first order time convergence proven in Theorem 1.

k	5	6	7	8	9	10
m_{LT}	1.0923	1.0438	1.022	1.011	1.0055	1.0028

8.2. **Vortex detection.** We now perform our simulation with $T = 5$ and time step size $\tau = 0.001$ so that $N = T/\tau$, denoting by $(U_n)_{0\leq n\leq N}$ the numerical solution obtained by the numerical scheme (LT) with $U_0 = P_h\psi_0$, and $\omega = 30$. We observe vortex nucleation in a similar way as [19]. In order to numerically track these vortices, we compute the approximation of the pseudo-vorticity $\omega_h(U^n)$ as described in Proposition 3 and we numerically detect the local extrema of the fiel $|\omega_h(U^n)|$. We plot the results obtained at final time $T = 5$ in Figure 3. More numerical experiments will be performed in a forthcoming work in various settings of physical relevance.

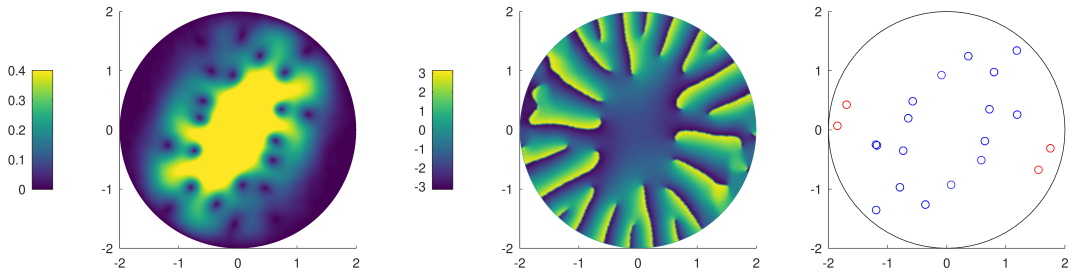

FIGURE 3. Plots of the density $|U^N|$, of the phase $\arg(U^N) \in [-\pi, \pi[$ and of the vortex detection algorithm results (from left to right).

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