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UNIFORMLY ACCURATE TIME-SPLITTING SCHEMES FOR NLS IN THE SEMICLASSICAL LIMIT

PHILIPPE CHARTIER, LOÏC LE TREUST, AND FLORIAN MÉHATS

ABSTRACT. We construct new numerical methods for the nonlinear Schrödinger equation in the semiclassical limit. We introduce time-splitting schemes for a phase-amplitude reformulation of the equation where the dimensionless Planck constant is not a singular parameter anymore. Our methods have an accuracy which is spectral in space, of second or fourth-order in time, and independent of the Planck constant before the formation of caustics. The scheme of second-order preserves exactly the L^2 norm of the solution, as the flow of the nonlinear Schrödinger equation does. In passing, we introduce a new time-splitting method for the eikonal equation, whose precision is spectral in space and of second or fourth-order in time.

1. Introduction

1.1. **Motivation.** We consider the solution $\Psi^\varepsilon : \mathbb{R}_+ \times \mathbb{R}^d \rightarrow \mathbb{C}$, $d \geq 1$ of the following nonlinear Schrödinger (NLS) equation:

$$i\varepsilon \partial_t \Psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \Psi^\varepsilon + |\Psi^\varepsilon|^2 \Psi^\varepsilon \quad (1.1)$$

where $\varepsilon > 0$ is the semiclassical parameter. The initial datum is assumed to be of the form

$$\Psi^\varepsilon(0, \cdot) = A_0(\cdot) e^{iS_0(\cdot)/\varepsilon}, \quad (1.2)$$

with

$$\|A_0\|_{L^2(\mathbb{R}^d)} = 1.$$

Note that the L^2 norm, the energy and the momentum of $\Psi^\varepsilon(0, \cdot)$ are preserved by the flow of equation (1.1) whenever $\Psi^\varepsilon(0, \cdot) \in H^1(\mathbb{R}^d)$, *i.e.*

$$\begin{aligned} \text{Mass: } & \frac{d}{dt} \|\Psi^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)}^2 = 0, \\ \text{Energy: } & \frac{d}{dt} \int_{\mathbb{R}^d} (\varepsilon^2 |\nabla \Psi^\varepsilon(t, x)|^2 + |\Psi^\varepsilon(t, x)|^4) dx = 0, \\ \text{Momentum: } & \frac{d}{dt} \varepsilon \operatorname{Im} \int_{\mathbb{R}^d} \overline{\Psi^\varepsilon(t, x)} \nabla \Psi^\varepsilon(t, x) dx = 0. \end{aligned} \quad (1.3)$$

Equation (1.1) appears in several domains of physics. In particular, it has been widely used for the description of the behavior of Bose-Einstein condensates as well as for the study of the propagation of lasers (see [31] for a detailed presentation of the

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physical context). In the semiclassical regime where the rescaled Planck constant ε is small, an asymptotic study of this equation provides relevant informations to describe the observables of Ψ^ε through the laws of hydrodynamics. We refer to [10] for a detailed presentation of the semiclassical analysis of the NLS equation and to [24] for a review of both theoretical and numerical issues.

Generally speaking, numerical methods for equation (1.1) exhibit an error of the form

$$\mathcal{O}\left(\frac{\Delta t^p + \Delta x^q}{\varepsilon^r}\right) \quad (1.4)$$

where Δt and Δx are the time and space steps and $p, q, r > 0$. Hence, in order to get a prescribed accuracy, one has to keep the ratios $\Delta t/\varepsilon^{r/p}$ and $\Delta x/\varepsilon^{r/q}$ small and constant. In practice, these constraints soon become impossible to satisfy as $\varepsilon \rightarrow 0$.

In this paper, we are interested in numerical schemes that are Uniformly Accurate (UA) with respect to ε . In other words, we look for methods that provide, for fixed time and space meshes, approximate solutions whose accuracy does not degrade as ε goes to 0, *i.e.* such that $r = 0$ in (1.4).

In the spirit of the WKB techniques (Wentzel, Kramers, Brillouin), we decompose Ψ^ε as the product of a slowly varying amplitude and a fast oscillating factor

$$\Psi^\varepsilon(t, \cdot) = A^\varepsilon(t, \cdot) e^{iS^\varepsilon(t, \cdot)/\varepsilon}. \quad (1.5)$$

From this point onwards, various choices are possible, depending for instance on whether A^ε is complex or not. In [21], taking $A^\varepsilon \in \mathbb{C}$, the following system of equations was considered

$$\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} + |A^\varepsilon|^2 = 0, \quad (1.6a)$$

$$\partial_t A^\varepsilon + \nabla S^\varepsilon \cdot \nabla A^\varepsilon + \frac{A^\varepsilon}{2} \Delta S^\varepsilon = \frac{i\varepsilon \Delta A^\varepsilon}{2} \quad (1.6b)$$

with

$$S^\varepsilon(0, \cdot) = S_0(\cdot) \text{ and } A^\varepsilon(0, \cdot) = A_0(\cdot)$$

and its analysis was performed with the tools of symmetrizable quasilinear hyperbolic systems. Under appropriate regularity assumptions, when $\varepsilon \rightarrow 0$, $A^\varepsilon \in \mathbb{C}$ and $S^\varepsilon \in \mathbb{R}$ converge to the solutions A^0 and S^0 of

$$\partial_t S^0 + \frac{|\nabla S^0|^2}{2} + |A^0|^2 = 0, \quad (1.7a)$$

$$\partial_t A^0 + \nabla S^0 \cdot \nabla A^0 + \frac{A^0}{2} \Delta S^0 = 0. \quad (1.7b)$$

Let us note that $(\rho, v) = (|A^0|^2, \nabla S^0)$ is solution of the following system of compressible Euler equations:

$$\partial_t v + v \cdot \nabla v + \nabla \rho = 0, \quad (1.8a)$$

$$\partial_t \rho + \operatorname{div}(\rho v) = 0. \quad (1.8b)$$

Remark 1.1. *The simplest way to relate the semiclassical limit of equation (1.1) to hydrodynamic equations is to use the Madelung transform [27]*

$$\Psi^\varepsilon(t, \cdot) = \sqrt{\rho^\varepsilon(t, \cdot)} e^{iS^\varepsilon(t, \cdot)/\varepsilon} \quad (1.9)$$

which amounts to choosing $A^\varepsilon \in \mathbb{R}_+$. Nevertheless, with this formulation, problems occur in the presence of vacuum, i.e. whenever ρ^ε vanishes, from both analytical and numerical points of view [16, 12].

An important difficulty raised by formulation (1.6) comes from the formation of caustics in finite time, see [10]. As a matter of fact, the solution of (1.6) may cease to be regular even if Ψ^ε is globally well-defined for $\varepsilon > 0$. To overcome this difficulty, Besse, Carles and Méhats [6] have introduced an equivalent system of equations with an asymptotically vanishing viscosity term in the eikonal equation (1.6a). This allows to get global existence for $\varepsilon > 0$ at least in the one-dimensional case. With these additional terms, (1.6) is now replaced by

$$\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} + |A^\varepsilon|^2 = \varepsilon^2 \Delta S^\varepsilon, \quad (1.10a)$$

$$\partial_t A^\varepsilon + \nabla S^\varepsilon \cdot \nabla A^\varepsilon + \frac{A^\varepsilon}{2} \Delta S^\varepsilon = \frac{i\varepsilon \Delta A^\varepsilon}{2} - i\varepsilon A^\varepsilon \Delta S^\varepsilon \quad (1.10b)$$

where

$$S^\varepsilon(0, x) = S_0(x) \text{ and } A^\varepsilon(0, x) = A_0(x), \quad x \in \mathbb{R}^d.$$

Let us emphasize that both systems (1.6) and (1.10) are equivalent to the original equation (1.1) in the following sense: as long as the solution $(S^\varepsilon, A^\varepsilon)$ of (1.6) (resp. (1.10)) is smooth, the function Ψ^ε defined by (1.5) solves (1.1).

Remark 1.2. *If we consider the WKB-ansatz (1.5), the invariants (1.3) become*

$$\begin{aligned} \text{Mass: } & \frac{d}{dt} \|A^\varepsilon\|_{L^2(\mathbb{R}^d)}^2 = 0, \\ \text{Energy: } & \frac{d}{dt} \int_{\mathbb{R}^d} (|\varepsilon \nabla A^\varepsilon + iA^\varepsilon \nabla S^\varepsilon|^2 + |A^\varepsilon|^4) dx = 0, \\ \text{Momentum: } & \frac{d}{dt} \operatorname{Im} \int_{\mathbb{R}^d} \overline{A^\varepsilon} (\varepsilon \nabla A^\varepsilon + iA^\varepsilon \nabla S^\varepsilon) dx = 0. \end{aligned} \quad (1.11)$$

Remark 1.3. *The Cole-Hopf transformation [20, Section 4.4.1]*

$$w^\varepsilon = \exp\left(-\frac{S^\varepsilon}{2\varepsilon^2}\right) - 1$$

transforms (1.10a) into

$$\partial_t w^\varepsilon - \frac{|A^\varepsilon|^2}{2\varepsilon^2} (w^\varepsilon + 1) = \varepsilon^2 \Delta w^\varepsilon.$$

for which the regularizing effect of the viscosity term becomes more apparent.

Since in (1.10), ε does not appear as a singular parameter anymore, this formulation is a good candidate upon which building UA schemes.

1.2. Existence, uniqueness and uniform boundedness results. Equation (1.1) has been widely studied and existence and uniqueness results can be found for instance in [15].

The first existence and uniqueness result for the solutions of (1.6) has been obtained by Grenier [21] using a reformulation of the problem in terms of symmetrizable quasilinear hyperbolic systems. Later [6], his proof has been adapted to (1.10).

Theorem 1.4 (Grenier, Besse-Carles-Méhats). *Let $\varepsilon_{\max} > 0$. Assume that (S_0, A_0) belongs to $H^{s+1}(\mathbb{R}^d) \times H^s(\mathbb{R}^d)$ where $s > d/2 + 1$. Then, there exist $T > 0$, independent of $\varepsilon \in (0, \varepsilon_{\max}]$ and a unique solution*

$$(S^\varepsilon, A^\varepsilon) \in C([0, T]; H^{s+1}(\mathbb{R}^d) \times H^s(\mathbb{R}^d))$$

of system of equations (1.6), resp. (1.10). Moreover, $(S^\varepsilon, A^\varepsilon)$ is bounded in

$$C([0, T]; H^{s+1}(\mathbb{R}^d) \times H^s(\mathbb{R}^d))$$

uniformly in ε and

$$\Psi^\varepsilon(t, \cdot) = A^\varepsilon(t, \cdot) e^{iS^\varepsilon(t, \cdot)/\varepsilon}$$

is the unique solution of (1.1) with the initial datum (1.2).

Remark 1.5. *Besse et al. [6] also proved that in the one-dimensional case, the solution of (1.10) is global in time under the assumptions of Theorem 1.4 and that $(S^\varepsilon, A^\varepsilon)$ is globally uniformly bounded.*

1.3. State of the art. Many numerical schemes have been introduced to approximate the solutions of (1.1): finite difference methods [33, 17, 1, 25], splitting methods [29, 32, 5, 26, 19, 18], relaxation schemes [4] and symplectic methods [30]. Nevertheless, none of these schemes is Uniformly Accurate (UA) with respect to ε . In particular, for the time-splitting method in the linear case, it is enough to keep the ratios $\Delta x/\varepsilon$ and $\Delta t^p/\varepsilon$ small enough to get a fixed precision on the wave function, where p is the order of the scheme [18, 2]. In the nonlinear framework, numerical experiments [19, 13, 3] suggest that more restrictive conditions have to be imposed after the appearance of the first caustics in (1.7). We refer to [19] for a theoretical study of the local error estimates for the semiclassical NLS equation.

However, as far as the observables (density, current, ...) are concerned, the situation is a little bit different. Bao, Jin, and Markowich [2] proved, using the Wigner transform, that the splitting method for the linear case is UA in time but not in space. More precisely, to get a prescribed accuracy on the observables, the quantities $\Delta x/\varepsilon$ and Δt have to be chosen small enough. These authors also performed extensive numerical simulations in both linear [2] and nonlinear [3] cases. Later on, Carles [11] studied the nonlinear case from a theoretical point of view. In particular, he proved that the same conclusion persists before the caustics for Hartree type nonlinearities and in the weakly nonlinear geometric optics case, *i.e.* when the nonlinearity is of the form $\varepsilon f(|\Psi^\varepsilon|^2)\Psi^\varepsilon$ instead of $f(|\Psi^\varepsilon|^2)\Psi^\varepsilon$.

As mentioned above, the main advantage of the WKB reformulations over (1.1) stems from the fact that the semiclassical parameter ε does not give rise to singular perturbations any longer. Hence, numerical schemes based on these systems of equations are more likely to be UA, at least prior to the appearance of caustics.

Previous attempts using WKB formulations suffer from several drawbacks, namely, either the presence of vacuum for the Madelung equation used in [16], or the occurrence of singularities in finite time for fixed $\varepsilon > 0$ in (1.6). To overcome this difficulty, UA schemes based on formulation (1.10) have been introduced in [6], taking advantage of the underlying hyperbolic structure and of the regularization properties of the parabolic term. Nevertheless, these schemes are built upon finite differences methods, are thus subject to CFL stability conditions and are of low order in time and space.

In this paper, in contrast with [6], we shall consider time-splitting methods for (1.10). In the next sections, it will become clear that splitting method indeed possess several advantages:

- (i) they do not suffer from stability restrictions on the time step;
- (ii) they are easy to implement;
- (iii) high-order of convergence in time can be attained as well as spectral convergence in space.

Note that the main difficulty to get high-order schemes comes from the fact that (1.10) contains Schrödinger as well as parabolic terms: we postpone the discussion of this point to the beginning of Section 3.

As a by-product, we also derive a new numerical scheme based on splitting techniques to approximate the solution of the Hamilton-Jacobi (eikonal) equation

$$\partial_t S + \frac{|\nabla S|^2}{2} = 0$$

based on the Cole-Hopf transform.

Finally, let us mention that we have chosen to focus here on the semiclassical regime of (1.1), referred to as supercritical (see [10]). Nevertheless, our approach is also relevant in other semiclassical regimes: either the linear Schrödinger equation with a given potential, or the weakly nonlinear geometric optics, where $|\Psi^\varepsilon|^2 \Psi^\varepsilon$ is replaced with $\varepsilon |\Psi^\varepsilon|^2 \Psi^\varepsilon$.

The outline of the paper is as follows. In Section 2, we introduce numerical schemes of order one and two in time that preserve exactly the L^2 norm. In Section 3, we present the time-splitting strategy that gives rise to schemes of high order in time. In Section 4, we present extensive numerical experiments comparing our methods to the Strang splitting method studied in [2, 3].

2. Second-order numerical scheme

The UA scheme that we now introduce is built upon splitting techniques (see for instance [28] for a general exposition). The first building block is the resolution of the eikonal equation. In the sequel, h denotes the time step.

2.1. The eikonal equation. Let us remind that the Cole-Hopf transformation

$$w^\varepsilon = \exp\left(-\frac{S^\varepsilon}{2\varepsilon^2}\right) - 1$$

ensures that solving

$$\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} = \varepsilon^2 \Delta S^\varepsilon, \quad S^\varepsilon(0, \cdot) = S_0(\cdot), \quad (2.1)$$

is equivalent to solving the heat equation

$$\partial_t w^\varepsilon = \varepsilon^2 \Delta w^\varepsilon, \quad w^\varepsilon(0, \cdot) = \exp\left(-\frac{S_0(\cdot)}{2\varepsilon^2}\right) - 1, \quad (2.2)$$

(see Remark 1.3).

Due to the limitations of the floating-point representation, it is completely inaccurate to solve (2.1) using (2.2) for small values of ε . To overcome this difficulty,

we split the nonviscous eikonal equation

$$\partial_t S + \frac{|\nabla S|^2}{2} = 0, \quad S(0, \cdot) = S_0(\cdot), \quad (2.3)$$

into two subequations, at each time step; the parabolic term $\varepsilon^2 \Delta S$ will be dealt with separately. The key idea is to allow S to be a complex-valued function despite the fact that the solutions of equations (1.6a), (1.10a), (2.1) and (2.3) take their values in \mathbb{R} .

First flow: let us define ϕ_h^1 as the exact flow at time $h \in \mathbb{R}$ of equation

$$\partial_t S + \frac{\nabla S \cdot \nabla S}{2} - i\Delta S = 0 \quad (2.4)$$

where $\nabla S \cdot \nabla S = \sum_{k=1}^d (\partial_k S)^2$. This equation can be solved thanks to the following modified Cole-Hopf transformation

$$w = \exp\left(\frac{iS}{2}\right) - 1$$

leading to

$$i\partial_t w = -\Delta w, \quad w(0, \cdot) = \exp\left(\frac{iS(0, \cdot)}{2}\right) - 1, \quad (2.5)$$

solved in the Fourier space and

$$S(h, \cdot) - S(0, \cdot) = -2i \log\left(1 + \frac{w(h, \cdot) - w(0, \cdot)}{w(0, \cdot) + 1}\right).$$

Remark 2.1. *This formula is well-defined whenever*

$$\left\| \frac{w(h, \cdot) - w(0, \cdot)}{w(0, \cdot) + 1} \right\|_{L^\infty} < 1,$$

a condition ensured as soon as h is small enough.

Second flow: ϕ_h^2 is the exact flow at time $h \in \mathbb{R}$ of the free Schrödinger equation

$$\partial_t S + i\Delta S = 0. \quad (2.6)$$

We are now able to define time-splitting schemes for equation (2.3). In particular, the *Lie-Trotter splitting formula*,

$$\text{Re } \phi_h^1 \circ \phi_h^2 \quad (2.7)$$

gives us an approximation of first-order in time of the solution of (2.3) (which is real-valued) while the *Strang splitting formula*

$$\text{Re } \phi_{h/2}^1 \circ \phi_h^2 \circ \phi_{h/2}^1 \quad (2.8)$$

provides a second-order method.

2.2. **Numerical schemes for system of equations (1.10).** We are now in position to introduce our numerical schemes. To this aim, we split system (1.10)

$$\begin{aligned}\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} + |A^\varepsilon|^2 &= \varepsilon^2 \Delta S^\varepsilon, \\ \partial_t A^\varepsilon + \nabla S^\varepsilon \cdot \nabla A^\varepsilon + \frac{A^\varepsilon}{2} \Delta S^\varepsilon &= \frac{i\varepsilon \Delta A^\varepsilon}{2} - i\varepsilon A^\varepsilon \Delta S^\varepsilon,\end{aligned}$$

into four subsystems.

First flow: Let us define φ_h^1 as the approximate flow at time $h \in \mathbb{R}$ of the system of equations:

$$\partial_t S + \frac{|\nabla S|^2}{2} = 0, \quad (2.9a)$$

$$\partial_t A + \nabla S \cdot \nabla A + \frac{A}{2} \Delta S = \frac{i\Delta A}{2}. \quad (2.9b)$$

The eikonal equation (2.9a) is solved according to Sec. 2.1. Equation (2.9b) is dealt with by noticing that $w = A \exp(iS)$ satisfies the free Schrödinger equation

$$i\partial_t w = -\frac{1}{2}\Delta w.$$

Second flow: φ_h^2 is the exact flow at time $h \in \mathbb{R}$ of

$$\partial_t S = 0, \quad (2.10a)$$

$$\partial_t A = \frac{i(\varepsilon - 1)\Delta A}{2} \quad (2.10b)$$

solved in the Fourier space.

Third flow: φ_h^3 is the exact flow at time $h \in \mathbb{R}$ of

$$\partial_t S = -|A|^2, \quad (2.11a)$$

$$\partial_t A = 0. \quad (2.11b)$$

Fourth flow: φ_h^4 is the exact flow at time $h \in \mathbb{R}_+$ of

$$\partial_t S = \varepsilon^2 \Delta S, \quad (2.12a)$$

$$\partial_t A = -i\varepsilon A \Delta S. \quad (2.12b)$$

Equation (2.12a) is solved in the Fourier space and the solution of (2.12b) is

$$A(h, \cdot) = \exp(-i\varepsilon^{-1}(S(h, \cdot) - S(0, \cdot))) A(0, \cdot).$$

Remark that φ_h^4 gathers the terms of (1.10) which are not in (1.6) and can thus be viewed as a regularizing flow.

Remark 2.2. *Let us stress that φ_h^4 is not defined for h such that $\operatorname{Re} h < 0$. As a matter of fact, the propagator $e^{z\Delta}$ is well-defined, in the distributional sense, if and only if $\operatorname{Re}(z) \geq 0$.*

We consider now the following methods for (1.10)

$$\varphi_h^1 \circ \varphi_h^2 \circ \varphi_h^3 \circ \varphi_h^4 \quad (2.13)$$

and

$$\varphi_{h/2}^1 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^3 \circ \varphi_h^4 \circ \varphi_{h/2}^3 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^1. \quad (2.14)$$

Standard results on splitting schemes [22] straightforwardly lead to the following local error estimates, inducing respectively global orders one and two for (2.13) and (2.14).

Proposition 2.3. *Assume that $(A_0, S_0) \in H^s(\mathbb{R}^d) \times H^{s+1}(\mathbb{R}^d)$ for a large enough s . Then, the following local error estimates hold true:*

$$\begin{aligned} \|\varphi_h^1 \circ \varphi_h^2 \circ \varphi_h^3 \circ \varphi_h^4(S_0, A_0) - (S^\varepsilon(h, \cdot), A^\varepsilon(h, \cdot))\|_{L^2} &\leq Ch^2 \\ \|\varphi_{h/2}^1 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^3 \circ \varphi_h^4 \circ \varphi_{h/2}^3 \circ \varphi_{h/2}^2 \circ \varphi_{h/2}^1(S_0, A_0) - (S^\varepsilon(h, \cdot), A^\varepsilon(h, \cdot))\|_{L^2} &\leq Ch^3 \end{aligned}$$

where C does not depend on $\varepsilon \in [0, \varepsilon_{\max}]$ and $(S^\varepsilon, A^\varepsilon)$ is the solution of system (1.10).

Remark 2.4. *It is worth mentioning that both schemes preserve exactly the L^2 norm of A since all φ_h^1 , φ_h^2 , φ_h^3 and φ_h^4 do so.*

3. Fourth-order numerical scheme

The splitting of (1.10) into the four flows (2.9), (2.10), (2.11), (2.12) proposed in the previous section is incompatible with splitting methods of order higher than 2 with real-valued coefficients. Indeed, it is known that such methods involve at least one negative time step for each part of the splitting (see for instance [7]). Therefore, we cannot build such a scheme for (1.10) because of its time irreversibility.

To circumvent this difficulty, it is possible to use splitting methods with complex coefficients [14, 8, 9, 23]. Let us point out the main restrictions on the coefficients in order for the methods to be well-defined. For obvious consistency reasons, if a flow φ_h is used with complex coefficients, then both $\varphi_{\alpha h}$ and $\varphi_{\beta h}$ with $\operatorname{Re} \alpha > 0$ and $\operatorname{Im} \beta < 0$ will appear. Hence, the flows φ_h^1 of (2.9) and φ_h^2 of (2.10) containing Schrödinger type terms have to be integrated with only real-valued coefficients, otherwise some parts of the splitting would be ill-posed. Moreover, φ_h^4 of (2.12) contains parabolic terms and it should be used with coefficients with nonnegative real part. In this section, we introduce a four-flow complex splitting method taking into account all these constraints.

The main remaining problem originates from the non-analytic character of the nonlinearity appearing in the flow φ_h^3 of (2.11). To overcome it, we split the real and imaginary part of A^ε as in [8].

Although we content ourselves in the sequel with a fourth-order scheme, let us emphasize that the strategy adopted here is amenable to higher orders.

3.1. The new splitting scheme. We commence from the original system (1.10)

$$\begin{aligned} \partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} + |A^\varepsilon|^2 &= \varepsilon^2 \Delta S^\varepsilon, \\ \partial_t A^\varepsilon + \nabla S^\varepsilon \cdot \nabla A^\varepsilon + \frac{A^\varepsilon}{2} \Delta S^\varepsilon &= \frac{i\varepsilon \Delta A^\varepsilon}{2} - i\varepsilon A^\varepsilon \Delta S^\varepsilon \end{aligned}$$

and rewrite it (following the steps exposed in [8]) in term of the unknowns $A_1^\varepsilon = \text{Re } A^\varepsilon$, $A_2^\varepsilon = \text{Im } A^\varepsilon$ and S^ε :

$$\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} + (A_1^\varepsilon)^2 + (A_2^\varepsilon)^2 = \varepsilon^2 \Delta S^\varepsilon, \quad (3.1a)$$

$$\left(\partial_t + \nabla S^\varepsilon \cdot \nabla + \frac{\Delta S^\varepsilon}{2} \right) \begin{pmatrix} A_1^\varepsilon \\ A_2^\varepsilon \end{pmatrix} = -i\varepsilon \sigma_2 \left(\frac{\Delta}{2} - \Delta S^\varepsilon \right) \begin{pmatrix} A_1^\varepsilon \\ A_2^\varepsilon \end{pmatrix} \quad (3.1b)$$

in order for the nonlinearity $(A_1^\varepsilon)^2 + (A_2^\varepsilon)^2$ to be an analytic function of A_1^ε and A_2^ε . The matrix σ_2 is here the second Pauli matrix

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

so that $P\sigma_2P = \sigma_3$ with

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad P = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\sigma_2 + \sigma_3). \quad (3.2)$$

Let

$$V^\varepsilon = \begin{pmatrix} v_1^\varepsilon \\ v_2^\varepsilon \end{pmatrix} = P \begin{pmatrix} A_1^\varepsilon \\ A_2^\varepsilon \end{pmatrix}.$$

System (3.1) becomes

$$\partial_t S^\varepsilon + \frac{|\nabla S^\varepsilon|^2}{2} - 2iv_1^\varepsilon v_2^\varepsilon = \varepsilon^2 \Delta S^\varepsilon, \quad (3.3a)$$

$$\left(\partial_t + \nabla S^\varepsilon \cdot \nabla + \frac{\Delta S^\varepsilon}{2} \right) V^\varepsilon = -i\varepsilon \sigma_3 \left(\frac{\Delta}{2} - \Delta S^\varepsilon \right) V^\varepsilon. \quad (3.3b)$$

We are now in position to define a four-flow splitting which is compatible with complex coefficients.

First flow: Let us define $\tilde{\varphi}_h^1$ as the approximate flow at time $h \in \mathbb{R}$ of:

$$\partial_t S + \frac{\nabla S \cdot \nabla S}{2} = 0, \quad (3.4a)$$

$$\partial_t V + \nabla S \cdot \nabla V + \frac{\Delta S}{2} V = \frac{i\Delta V}{2}. \quad (3.4b)$$

To solve (3.4a), we use the following fourth-order time-splitting from [34]

$$\phi_{\alpha_1 h}^1 \circ \phi_{\alpha_2 h}^2 \circ \phi_{\alpha_3 h}^1 \circ \phi_{\alpha_4 h}^2 \circ \phi_{\alpha_5 h}^1 \circ \phi_{\alpha_6 h}^2 \circ \phi_{\alpha_7 h}^1, \quad (3.5)$$

with coefficients $\alpha_1, \dots, \alpha_7$ defined by

$$\begin{aligned} \alpha_1 = \alpha_7 &= \frac{1}{2(2 - 2^{1/3})}, & \alpha_3 = \alpha_5 &= 0.5 - \alpha_1, \\ \alpha_2 = \alpha_6 &= \frac{1}{2 - 2^{1/3}}, & \alpha_4 &= 1 - 2\alpha_2 \end{aligned} \quad (3.6)$$

and where the numerical flows ϕ_h^1 and ϕ_h^2 are those introduced in Sec. 2.1. To solve (3.4b), we proceed as for (2.9b).

Second flow: $\tilde{\varphi}_h^2$ is the exact flow at time $h \in \mathbb{R}$ of

$$\partial_t S = 0, \quad (3.7a)$$

$$\partial_t V = -\frac{i(\varepsilon \sigma_3 + \sigma_0) \Delta V}{2} \quad (3.7b)$$

solved in the Fourier space. Here σ_0 denotes the identity matrix.

Third flow: $\tilde{\varphi}_h^3$ is the exact flow at time $h \in \mathbb{R}$ of

$$\partial_t S = 2iv_1v_2, \quad (3.8a)$$

$$\partial_t V = 0. \quad (3.8b)$$

Fourth flow: $\tilde{\varphi}_h^4$ is the exact flow at time $h \in \{z \in \mathbb{C}, \operatorname{Re} z \geq 0\}$ of

$$\partial_t S = \varepsilon^2 \Delta S, \quad (3.9a)$$

$$\partial_t V = i\varepsilon\sigma_3 V \Delta S. \quad (3.9b)$$

We will see below that in the complex splitting method that we use, the coefficients related to $\tilde{\varphi}_h^4$ are complex so that S , v_1 and v_2 are complex-valued functions.

3.2. Splitting scheme of fourth-order for system (1.10). We define below a complex splitting method whose coefficients related to $\tilde{\varphi}_h^4$ have positive real part whereas those associated with $\tilde{\varphi}_h^1$ and $\tilde{\varphi}_h^2$ are real-valued.

The simplest way to get a fourth-order time-splitting scheme for four flows is to compose several times a fourth-order time-splitting for two flows: using the same time-splitting scheme as in (3.5), we define the following fourth-order schemes (for $h \in \mathbb{R}$):

$$\tilde{\varphi}_h^{12} = \tilde{\varphi}_{\alpha_1 h}^2 \circ \tilde{\varphi}_{\alpha_2 h}^1 \circ \tilde{\varphi}_{\alpha_3 h}^2 \circ \tilde{\varphi}_{\alpha_4 h}^1 \circ \tilde{\varphi}_{\alpha_5 h}^2 \circ \tilde{\varphi}_{\alpha_6 h}^1 \circ \tilde{\varphi}_{\alpha_7 h}^2$$

for the system of equations

$$\begin{aligned} \partial_t S + \frac{\nabla S \cdot \nabla S}{2} &= 0, \\ \partial_t V + \nabla S \cdot \nabla V + \frac{\Delta S}{2} V &= -i\varepsilon\sigma_3 \frac{\Delta V}{2}. \end{aligned}$$

and

$$\tilde{\varphi}_h^{123} = \tilde{\varphi}_{\alpha_1 h}^{12} \circ \tilde{\varphi}_{\alpha_2 h}^3 \circ \tilde{\varphi}_{\alpha_3 h}^{12} \circ \tilde{\varphi}_{\alpha_4 h}^3 \circ \tilde{\varphi}_{\alpha_5 h}^{12} \circ \tilde{\varphi}_{\alpha_6 h}^3 \circ \tilde{\varphi}_{\alpha_7 h}^{12},$$

for the system of equations

$$\begin{aligned} \partial_t S + \frac{\nabla S \cdot \nabla S}{2} - 2iv_1v_2 &= 0, \\ \partial_t V + \nabla S \cdot \nabla V + \frac{\Delta S}{2} V &= -i\varepsilon\sigma_3 \frac{\Delta V}{2}. \end{aligned}$$

The coefficients $\alpha_1, \dots, \alpha_7$ are defined by (3.6). Since $\tilde{\varphi}_h^4$ is not reversible, we cannot use the scheme (3.5) anymore to define our four-flow method, given that α_3, α_4 and α_5 are negative. To avoid this problem, we use a complex splitting method of Blanes *et al.* [8]:

$$\tilde{\varphi}_h^{1234} = \tilde{P} (\tilde{\varphi}_{\beta_1 h}^4 \circ \tilde{\varphi}_{\beta_2 h}^{123} \circ \tilde{\varphi}_{\beta_3 h}^4 \circ \tilde{\varphi}_{\beta_4 h}^{123} \circ \tilde{\varphi}_{\beta_5 h}^4 \circ \tilde{\varphi}_{\beta_6 h}^{123} \circ \tilde{\varphi}_{\beta_7 h}^4 \circ \tilde{\varphi}_{\beta_8 h}^{123} \circ \tilde{\varphi}_{\beta_9 h}^4) \tilde{P} \quad (3.10)$$

where

$$\tilde{P} = \begin{pmatrix} 1 & 0 \\ 0 & P \end{pmatrix},$$

P is defined in (3.2) and

$$\begin{aligned}\beta_1 &= \beta_9 = 0.060078275263542357774 - 0.060314841253378523039i, \\ \beta_2 &= \beta_8 = 0.18596881959910913140, \\ \beta_3 &= \beta_7 = 0.27021183913361078161 + 0.15290393229116195895i, \\ \beta_4 &= \beta_6 = 0.5 - \beta_2 = 0.31403118040089086860, \\ \beta_5 &= 1 - 2\beta_1 - 2\beta_3 = 0.33941977120569372122 - 0.18517818207556687181i.\end{aligned}$$

Observe that all the coefficients $\beta_1, \beta_3, \beta_5, \beta_7$ and β_9 for the irreversible flow $\tilde{\varphi}_h^4$ have a positive real part and all the coefficients $\beta_2, \beta_4, \beta_6$ and β_8 for the flow $\tilde{\varphi}_h^{123}$ containing all the Schrödinger terms are real-valued.

Following [8], we state without proof the following proposition.

Proposition 3.1. *Assume that $(A_0, S_0) \in H^s(\mathbb{R}^d) \times H^{s+1}(\mathbb{R}^d)$ for a large enough s . Then, the following error bound holds true*

$$\|\tilde{\varphi}_h^{1234}(S_0, \operatorname{Re} A_0, \operatorname{Im} A_0) - (S^\varepsilon(h, \cdot), \operatorname{Re} A^\varepsilon(h, \cdot), \operatorname{Im} A^\varepsilon(h, \cdot))\|_{L^2} \leq Ch^5$$

where C does not depend on $\varepsilon \in [0, \varepsilon_{\max}]$ and $(S^\varepsilon, A^\varepsilon)$ is the solution of system of equations (1.10).

Let us remark that since S^ε takes complex values, the L^2 norm of A^ε is not exactly conserved by the flows $\tilde{\varphi}_h^1$ and $\tilde{\varphi}_h^4$. We stress that the function S^ε is not projected on the set of real-valued functions after each flow, as it was done in Section 2, since it would reduce the order of convergence.

4. Numerical experiments

In this part, we illustrate the behavior of the schemes (2.14) and (3.10) introduced in Sections 2 and 3 and compare their properties to those of the Strang splitting method [3] for (1.1). As mentioned in the introduction, quadratic observables have some peculiarities for this problem. For this reason, the convergence properties of the different schemes will be illustrated separately, on the one hand for the functions $S^\varepsilon, A^\varepsilon$ (resp. Ψ^ε for the Strang splitting scheme) and, on the other hand, for the density $\rho^\varepsilon = |A^\varepsilon|^2$ (resp. $\rho^\varepsilon = |\Psi^\varepsilon|^2$). We restrict ourselves to the one-dimensional periodic setting in which the equations studied remain unchanged.

We consider the following initial data:

$$\begin{aligned}A_0(x) &= \sin(x), & S_0(x) &= \sin(x)/2, \\ \Psi^\varepsilon(0, \cdot) &= A_0(\cdot)e^{iS_0(\cdot)/\varepsilon},\end{aligned}\tag{4.1}$$

where $x \in \mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$, for which caustics appear numerically at time $T_c = 0.5$. In our simulations, the semiclassical parameter ε varies from 1 to 2^{-12} .

The numerical solutions $(S^\varepsilon, A^\varepsilon)$, resp. Ψ^ε , are compared to corresponding reference solutions $(S_{ref}^\varepsilon, A_{ref}^\varepsilon)$, resp. Ψ_{ref}^ε , which, in the absence of analytical solutions, are respectively obtained thanks to our fourth order splitting method (3.10) and thanks to a splitting scheme of order 4 for (1.1) (see [34, 3]), with very small time and space steps. More precisely, to compute $(S_{ref}^\varepsilon, A_{ref}^\varepsilon)$, we have taken $N_x = 2^8$ and $h = 2^{-13}T_f$, and to compute Ψ_{ref}^ε , in order to fit with the constraints on the time step and on the space step

$$h \ll \varepsilon \text{ and } \Delta x \ll \varepsilon,$$

the space interval $[0, 2\pi]$ is discretized with $N_x = 2^{15}$ points and the time step is $h = 2^{-18}T_f$.

The various errors that are represented on the figures below are defined as follows:

$$err_{\rho^\varepsilon}(T) = \frac{\|\rho_{ref}^\varepsilon(T) - \rho^\varepsilon(T)\|_{L^1}}{\|\rho_{ref}^\varepsilon(T)\|_{L^1}}, \quad err_{\Psi^\varepsilon}(T) = \frac{\|\Psi_{ref}^\varepsilon(T) - \Psi^\varepsilon(T)\|_{L^2}}{\|\psi_{ref}^\varepsilon(T)\|_{L^2}},$$

and

$$err_{(S^\varepsilon, A^\varepsilon)}(T) = \left(\frac{\|S_{ref}^\varepsilon(T) - S^\varepsilon(T)\|_{L^2}^2 + \|A_{ref}^\varepsilon(T) - A^\varepsilon(T)\|_{L^2}^2}{\|S_{ref}^\varepsilon(T)\|_{L^2}^2 + \|A_{ref}^\varepsilon(T)\|_{L^2}^2} \right)^{1/2},$$

where

$$\|u\|_{L^1} = \Delta x \sum_{k=0}^{N_x-1} |u_k|, \quad \|u\|_{L^2} = \sqrt{\Delta x \sum_{k=0}^{N_x-1} |u_k|^2},$$

and $\rho_{ref}^\varepsilon(T) = |\Psi_{ref}^\varepsilon(T)|^2$. As far as the Strang splitting scheme is concerned, $\rho^\varepsilon(T) = |\Psi^\varepsilon(T)|^2$ whereas $\rho^\varepsilon(T) = |A^\varepsilon(T)|^2$ for our methods.

We first study qualitatively the dynamics, in order to guess what is the time of appearance of the caustics. Figures 1a and 1b represent the density $|A^\varepsilon|^2$ and the phase S^ε at times $T_f = 0.1, 0.3, 0.5, 0.6$ for $\varepsilon = 2^{-5}$. The caustics appear around $t = 0.5$. At time $t = 0.6$, oscillations at other scales than those of the phase can be observed in $|A^\varepsilon|^2$ whereas S^ε ceases to be smooth. These figures are obtained by using our scheme (2.14) with $N_x = 2^{11}$ and $N_t = T_f/h = 2^{13}$.

Let us now illustrate the behavior of the Strang splitting scheme for (1.1) at time $T_f = 0.1$ *i.e.* before the caustics. On Figures 2 and 3, errors on ρ^ε and Ψ^ε with respect to the time step h , for fixed $N_x = 2^9$, are represented and on Figures 4 to 5, errors with respect to Δx , for fixed $N_t = h/T_f = 2^{15}$, are represented. Regarding the observable $\rho^\varepsilon = |\Psi^\varepsilon|^2$, 2a, 2b, 4a and 4b corroborate the fact that the error behaves as

$$\mathcal{O}(h^2 + C_{\varepsilon, N} \Delta x^N)$$

where $N > 0$ and $C_{\varepsilon, N} \rightarrow +\infty$ as $\varepsilon \rightarrow 0$ [2, 3, 11]. This is in agreement with the results obtained by Carles [11] in the weakly nonlinear case before the caustics; however, our simulations suggest that this behavior persists in the supercritical case. If we observe the wave function, the situation is completely different: the Strang splitting scheme is not UA any more when $h \rightarrow 0$. Figures 3a, 3b, 5a and 5b indeed suggest that the error of Ψ^ε behaves like

$$\mathcal{O}\left(\frac{h^2}{\varepsilon} + C_{\varepsilon, N} \Delta x^N\right)$$

where $N > 0$ and $C_{\varepsilon, N} \rightarrow +\infty$ as $\varepsilon \rightarrow 0$.

Let us now focus on the experiments performed with our second and fourth-order methods, in the same situation. We start with the second-order scheme (2.14). Figures 6 and 7 represent the errors on ρ^ε and $(S^\varepsilon, A^\varepsilon)$ *w.r.t.* the time step h for a fixed $N_x = 2^7$. Figures 8 and 9 represent the errors *w.r.t.* Δx for fixed $N_t = h/T_f = 2^{13}$. All these figures illustrate the fact that our scheme is UA with respect to ε , for the quadratic observables as well as for the whole unknown $(S^\varepsilon, A^\varepsilon)$ itself. Figures 6 and 7 show that (2.14) is uniformly of order 2 in time, whereas Figures 8 and 9 show that the convergence is uniformly spectral in space.

Figures 10 to 13 illustrate the behavior of our fourth-order scheme (3.10) at $T_f = 0.1$: here again, it appears that, before the caustics, our method is UA with an order 4 in time and with spectral in space accuracy.

Finally, let us explore the behavior of the splitting methods after caustics, by observing the error on the density ρ^ε . Figures 14, 15, 16 and 17 present the same simulations as Figures 2, 4, 6 and 8, except that the final time is now $T_f = 0.6$, *i.e.* we illustrate the behaviors of Strang splitting method and of scheme (2.14) after the caustics. In that case, it appears that none of these methods is UA, neither in h , nor in Δx , with respect to ε . Concerning the Strang splitting scheme, this behavior was already reported in [13, 24]. Notice that, although it is not UA any longer, our scheme (2.14) still has second-order accuracy in time and spectral accuracy in space (with ε -dependent constants). Recall that the same scheme written on (1.6) would not be usable in the same situation, since S^ε ceases to be regular for $\varepsilon > 0$, after the formation of caustics.

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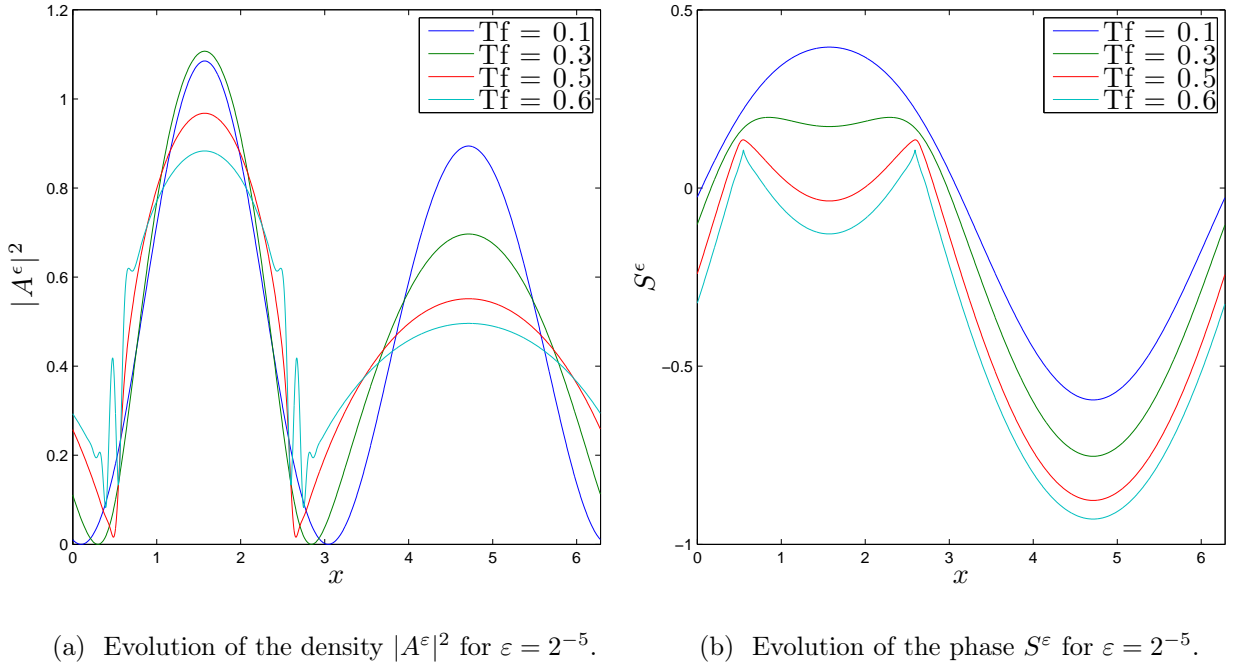
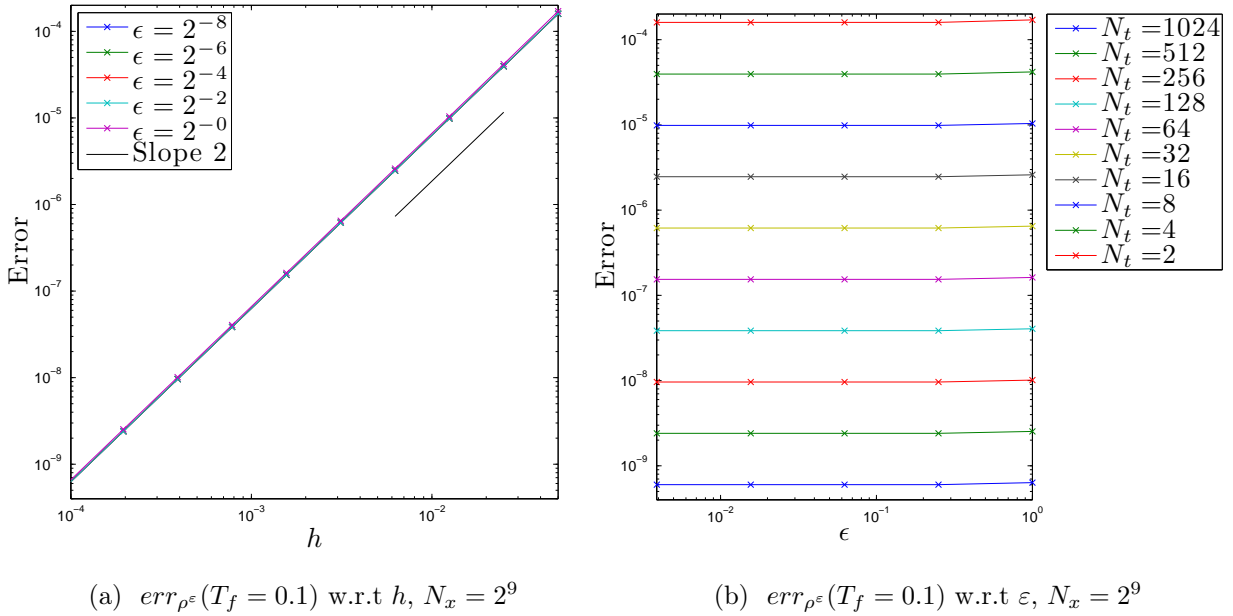


FIGURE 1. Evolution of the density and of the phase

FIGURE 2. Error on the density ρ^ϵ for the Strang splitting scheme for (1.1) before the caustics: dependence on ϵ and on the time step h .

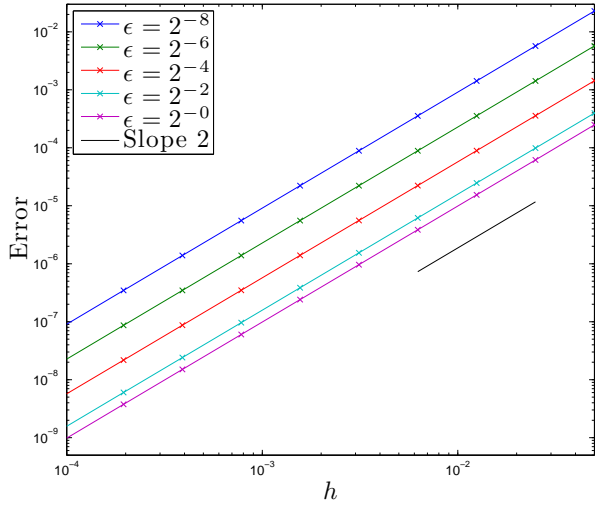
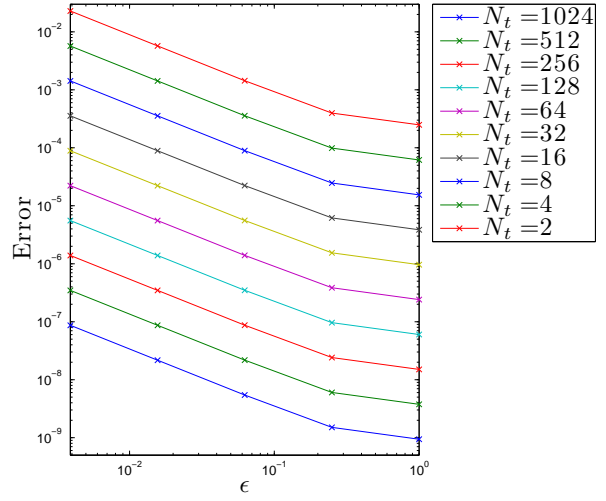
(a) $err_{\Psi^\varepsilon}(T_f = 0.1)$ w.r.t h , $N_x = 2^9$ (b) $err_{\Psi^\varepsilon}(T_f = 0.1)$ w.r.t ε , $N_x = 2^9$

FIGURE 3. Error on the wave function Ψ^ε for the Strang splitting scheme for (1.1) before the caustics: dependence on ε and on the time step h .

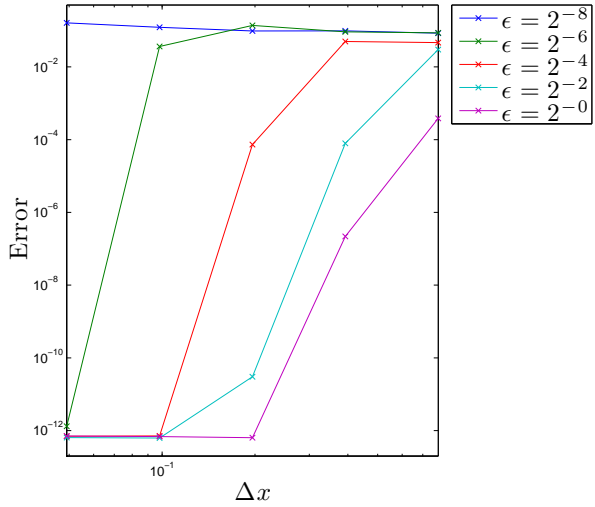
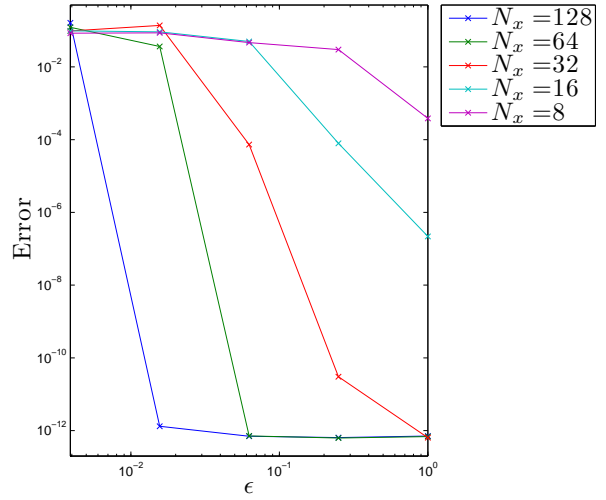
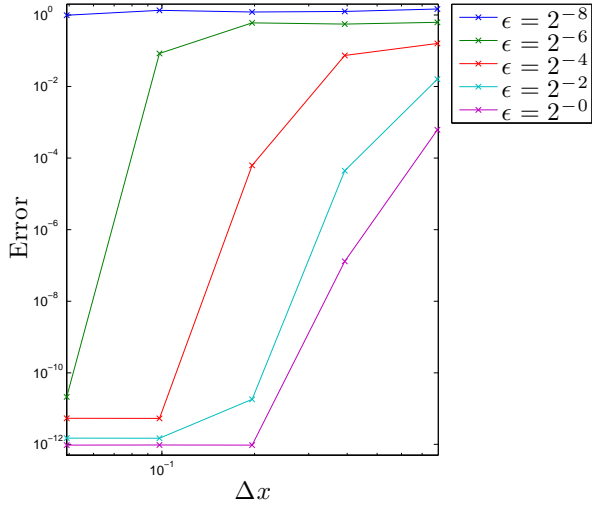
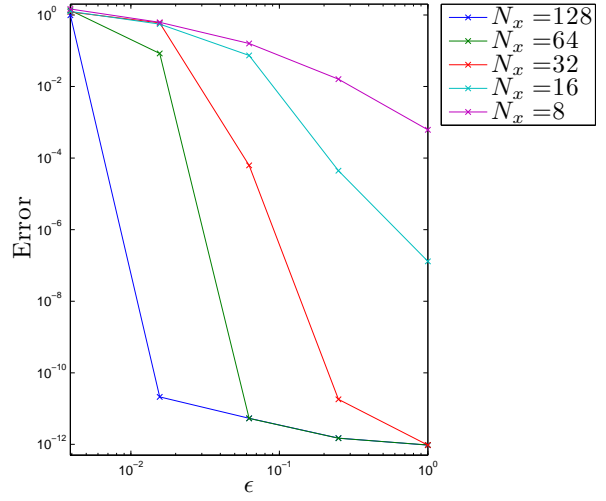
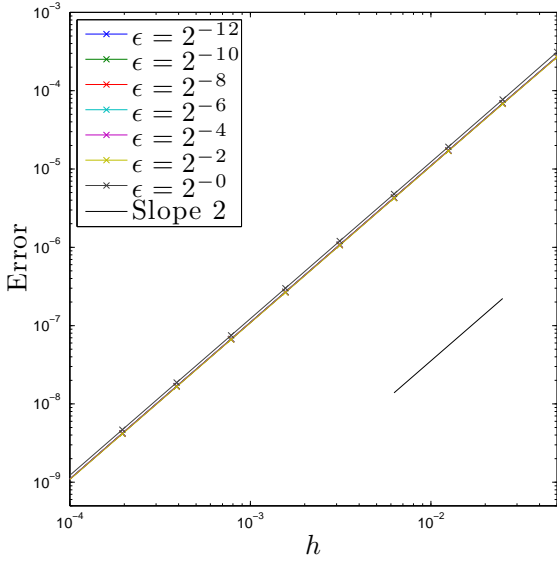
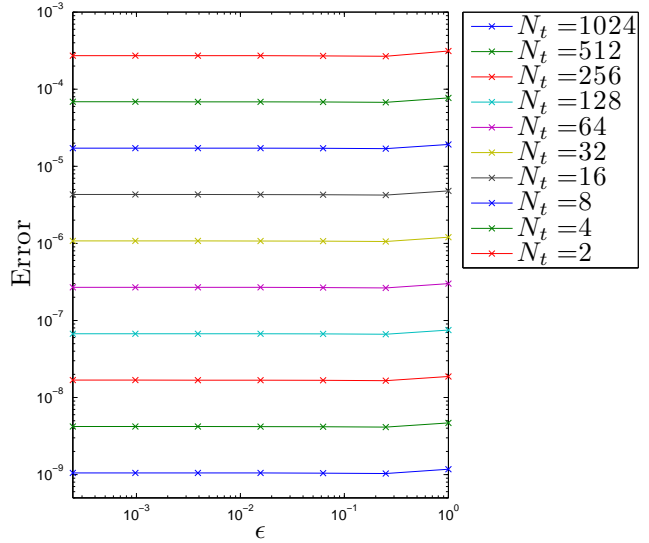
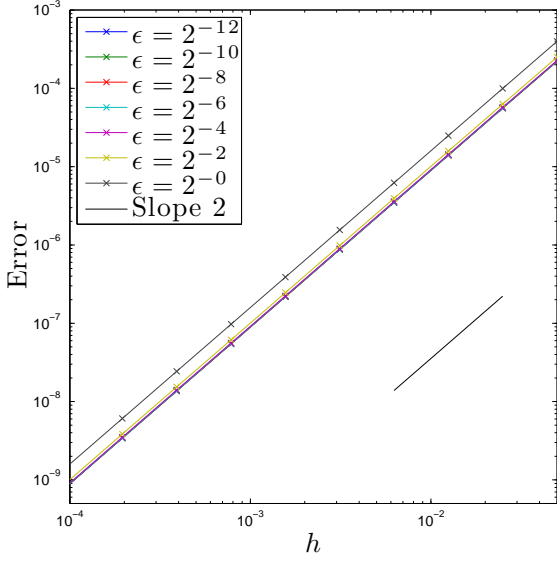
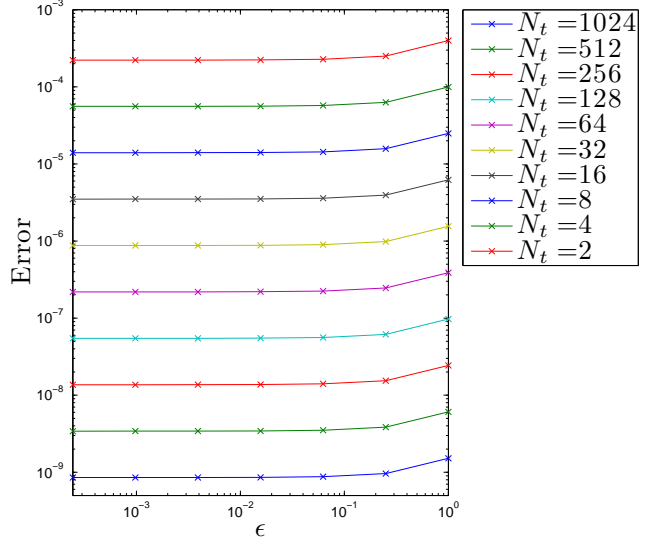
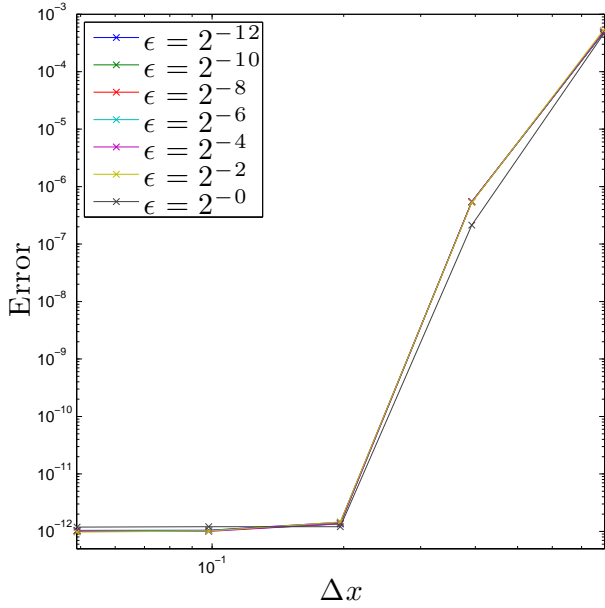
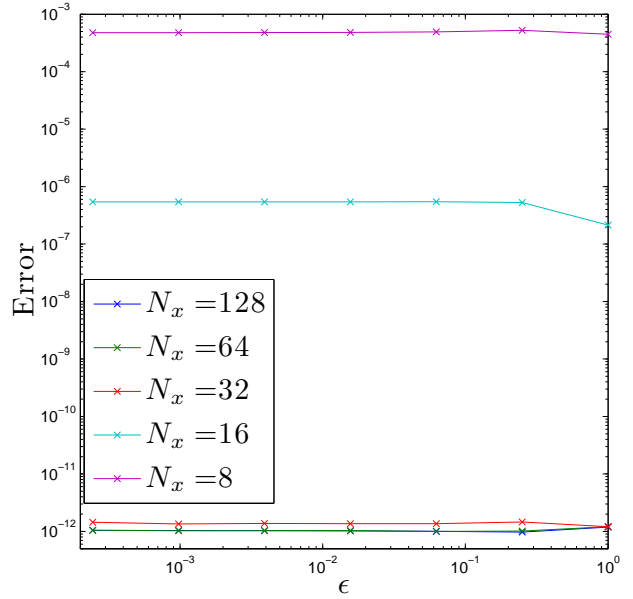
(a) $err_{\rho^\varepsilon}(T_f = 0.1)$ w.r.t Δx , $N_t = 2^{15}$ (b) $err_{\rho^\varepsilon}(T_f = 0.1)$ w.r.t ε , $N_t = 2^{15}$

FIGURE 4. Error on the density ρ^ε for the Strang splitting scheme for (1.1) before the caustics: dependence on ε and on Δx .

(a) $err_{\Psi^\varepsilon}(T_f = 0.1)$ w.r.t Δx , $N_t = 2^{15}$ (b) $err_{\Psi^\varepsilon}(T_f = 0.1)$ w.r.t ε , $N_t = 2^{15}$ FIGURE 5. Error on the wave function Ψ^ε for the Strang splitting scheme for (1.1) before the caustics: dependence on ε and on Δx .(a) $err_{\rho^\varepsilon}(T_f = 0.1)$ w.r.t h , $N_x = 2^7$ (b) $err_{\rho^\varepsilon}(T_f = 0.1)$ w.r.t ε , $N_x = 2^7$ FIGURE 6. Error on the density ρ^ε for the splitting scheme (2.14) of order 2 before the caustics: dependence on ε and on h .

(a) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t h , $N_x = 2^7$ (b) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t ϵ , $N_x = 2^7$ FIGURE 7. Error on (S^ϵ, A^ϵ) for the splitting scheme (2.14) of order 2 before the caustics: dependence on ϵ and on h .(a) $err_{\rho^\epsilon}(T_f = 0.1)$ w.r.t Δx , $N_t = 2^{15}$ (b) $err_{\rho^\epsilon}(T_f = 0.1)$ w.r.t ϵ , $N_t = 2^{15}$ FIGURE 8. Error on the density ρ^ϵ for the splitting scheme (2.14) of order 2 before the caustics: dependence on ϵ and on Δx .

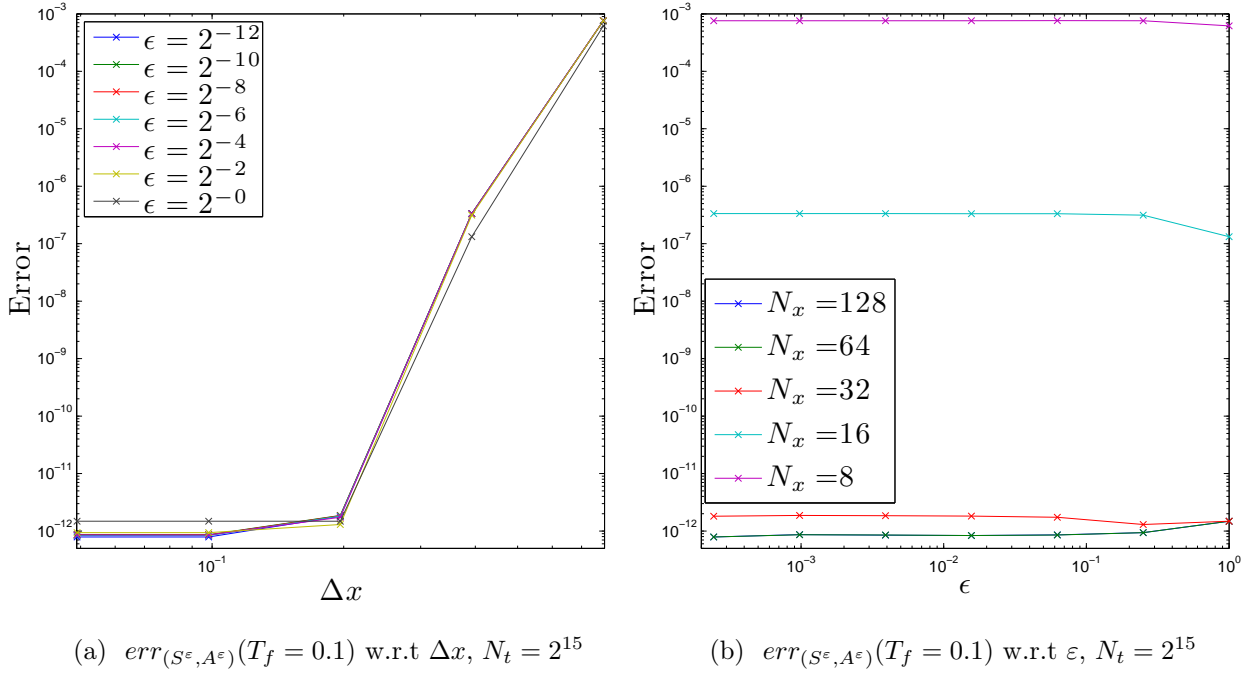


FIGURE 9. Error on (S^ϵ, A^ϵ) for the splitting scheme (2.14) of order 2 before the caustics: dependence on ϵ and on Δx .

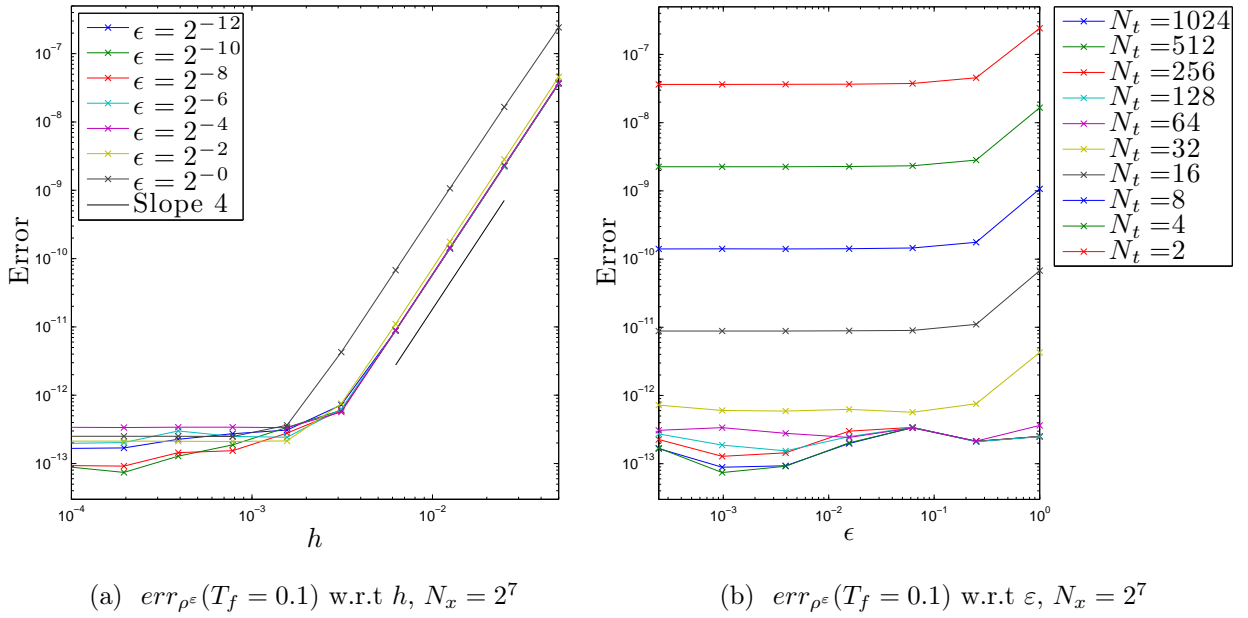
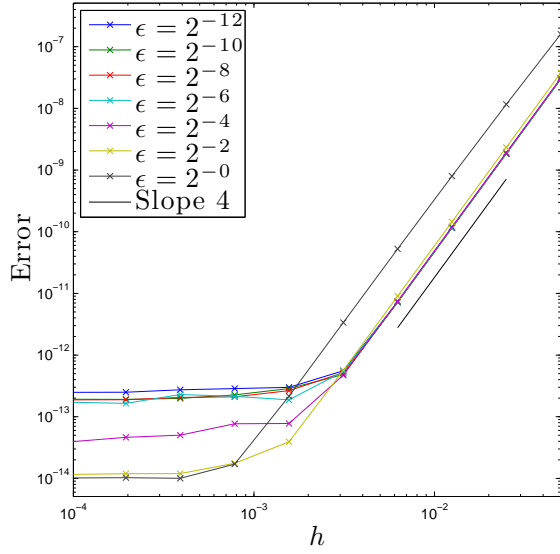
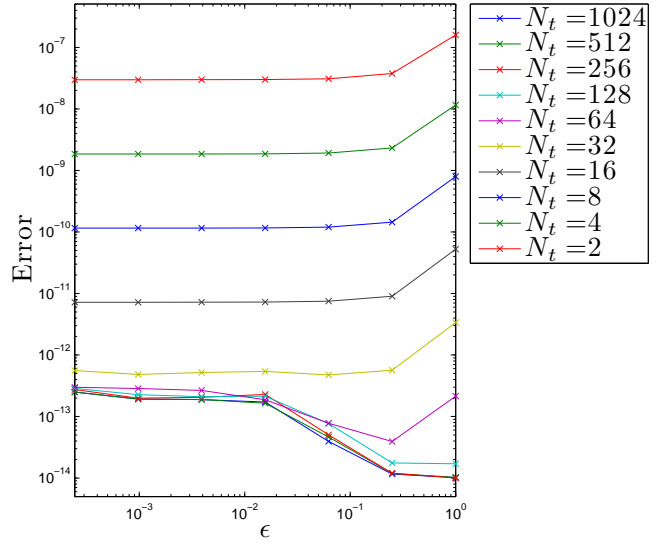
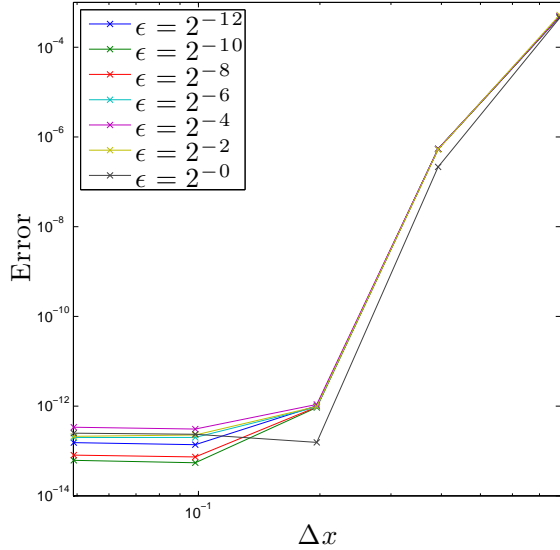
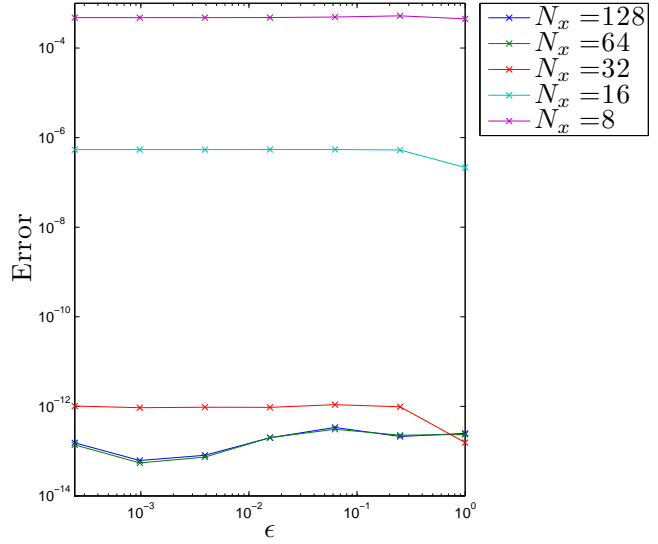
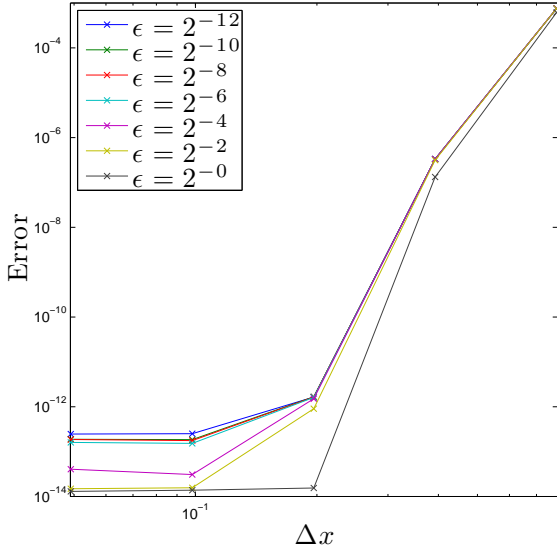
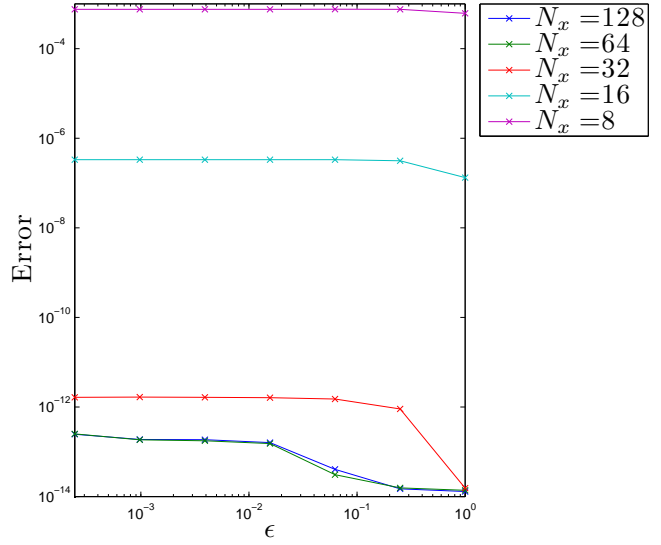
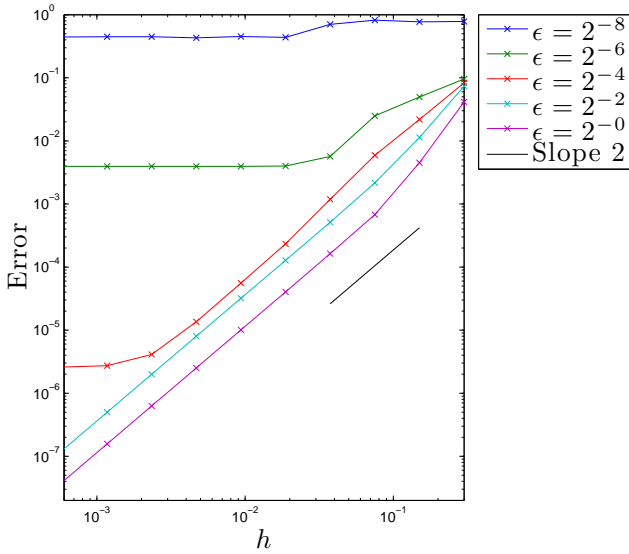
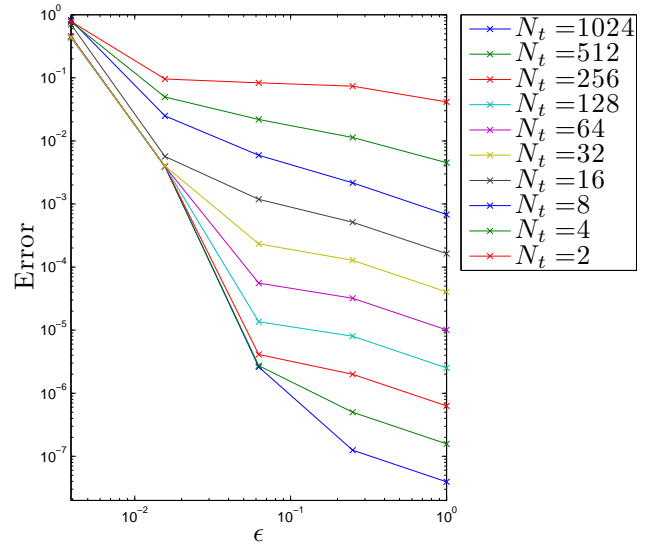


FIGURE 10. Error on the density ρ^ϵ for the splitting scheme (3.10) of order 4 before the caustics: dependence on ϵ and on h .

(a) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t h , $N_x = 2^7$ (b) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t ϵ , $N_x = 2^7$ FIGURE 11. Error on (S^ϵ, A^ϵ) for the splitting scheme (3.10) of order 4 before the caustics: dependence on ϵ and on h .(a) $err_{\rho^\epsilon}(T_f = 0.1)$ w.r.t Δx , $N_t = 2^{13}$ (b) $err_{\rho^\epsilon}(T_f = 0.1)$ w.r.t ϵ , $N_t = 2^{13}$ FIGURE 12. Error on ρ^ϵ for the splitting scheme (3.10) of order 4 before the caustics: dependence on ϵ and on Δx .

(a) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t Δx , $N_t = 2^{13}$ (b) $err_{(S^\epsilon, A^\epsilon)}(T_f = 0.1)$ w.r.t ϵ , $N_t = 2^{13}$ FIGURE 13. Error on (S^ϵ, A^ϵ) for the splitting scheme (3.10) of order 4 before the caustics: dependence on ϵ and on Δx .(a) $err_{\rho^\epsilon}(T_f = 0.6)$ w.r.t h , $N_x = 2^7$ (b) $err_{\rho^\epsilon}(T_f = 0.6)$ w.r.t ϵ , $N_x = 2^7$ FIGURE 14. Error on ρ^ϵ for the Strang splitting scheme for (1.1) after the caustics, dependence on ϵ and on h .

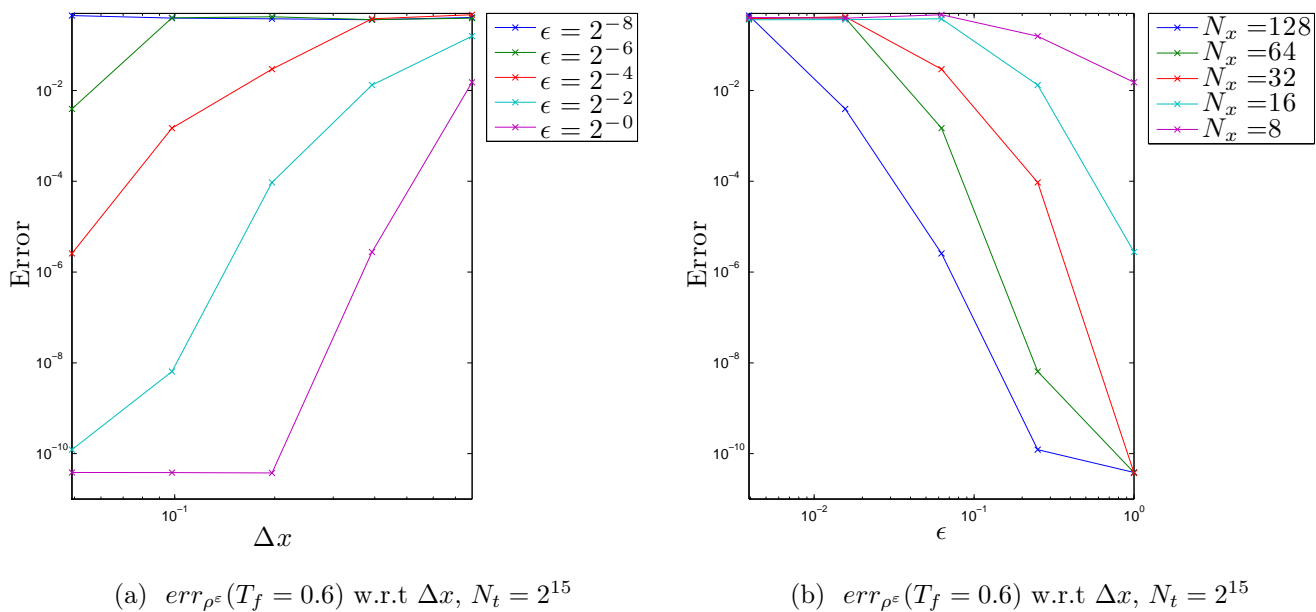


FIGURE 15. Error on ρ^ϵ for the Strang splitting scheme for (1.1) after the caustics, dependence on ϵ and on Δx .

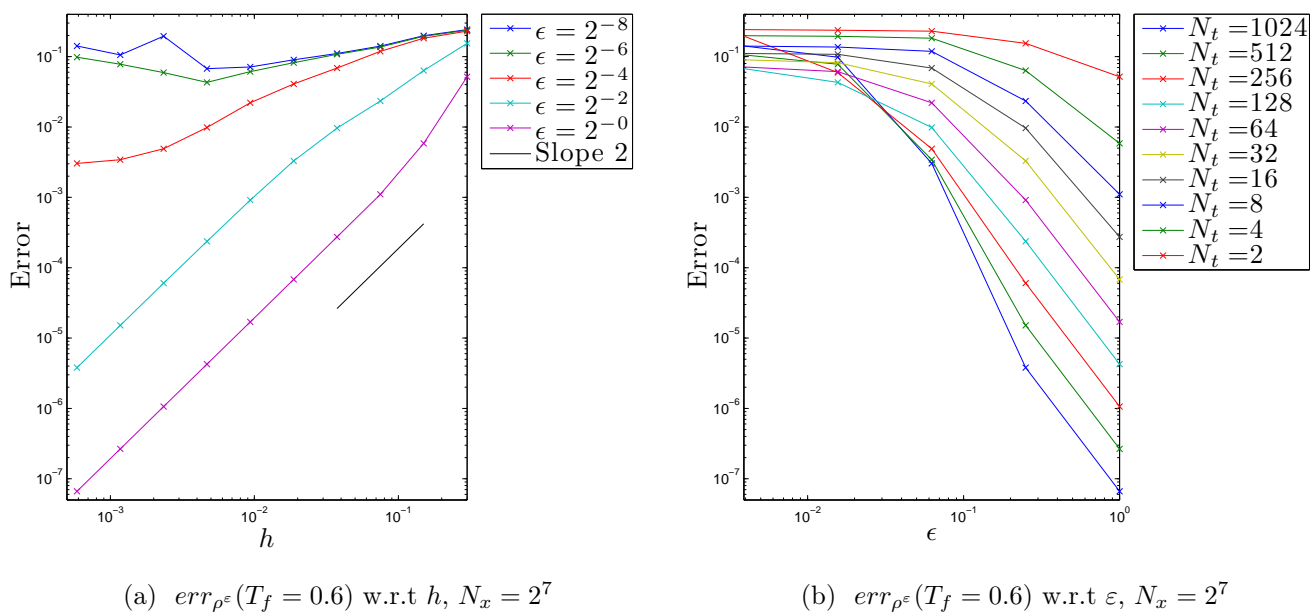
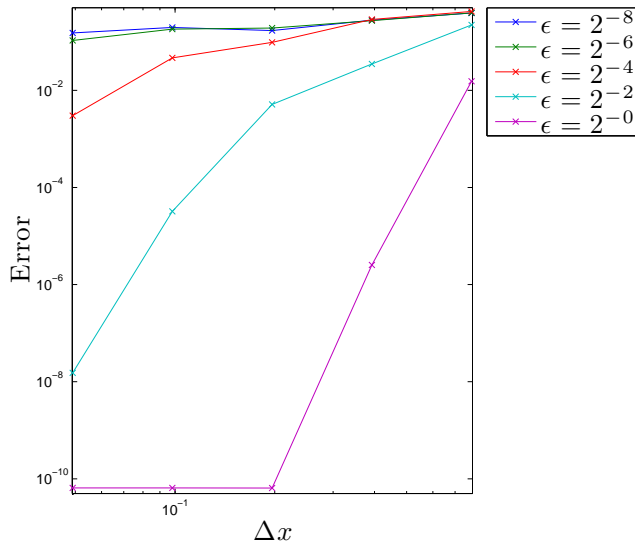
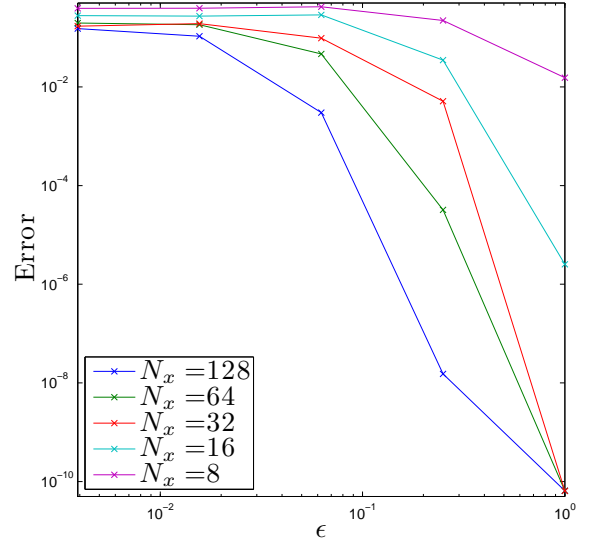


FIGURE 16. Error on ρ^ϵ for the splitting scheme (2.14) of order 2 after the caustics, dependence on ϵ and on h .

(a) $err_{\rho^\varepsilon}(T_f = 0.6)$ w.r.t Δx , $N_t = 2^{15}$ (b) $err_{\rho^\varepsilon}(T_f = 0.6)$ w.r.t ε , $N_t = 2^{15}$ FIGURE 17. Error on ρ^ε for the splitting scheme (2.14) of order 2 after the caustics, dependence on ε and on Δx .