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Convergence results for an inhomogeneous system arising in various high frequency approximations

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Summary. This paper is devoted to both theoretical and numerical study of a system involving an eikonal equation of Hamilton-Jacobi type and a linear conservation law as it comes out of the geometrical optics expansion of the wave equation or the semiclassical limit for the Schrödinger equation. We first state an existence and uniqueness result in the framework of viscosity and duality solutions. Then we study the behavior of some classical numerical schemes on this problem and we give sufficient conditions to ensure convergence. As an illustration, some practical computations are provided.

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1 Introduction

The aim of this paper is to give both a theoretical and numerical study of a one-dimensional system of two equations: a nonlinear Hamilton-Jacobi equation coupled with a linear transport equation. Such unusual systems naturally arise in two applications which will illustrate our results: geometrical optics for the wave equation, and semiclassical limit for the Schrödinger equation. Both theories involve a small parameter, and we are interested in computing approximations of the highly oscillating solutions emanating

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in the limit when this parameter goes to zero. One of the motivations for introducing such asymptotics is of numerical order: we replace the brute computation of highly oscillating functions by the study of a system of equations which takes their shape into account.

In the Schrödinger case, the small parameter is already present in the equations: it is the Planck constant. The semiclassical limit consists in studying the solution generated by initial data tuned to the wavelength equal to the Planck constant. Concerning the wave equation, we artificially introduce a small wavelength in the inital datum. In both cases, one seeks a solution u by means of an ansatz of the form $u(t,x) = A(t,x)\exp(ik\varphi(t,x))$, where φ is the phase of the wave, $A \geq 0$ its amplitude, and k its (high) frequency. We then perform an expansion in powers of k and, by considering the first two terms, we formally find that

– the phase φ is a solution to the so-called eikonal equation, which is usually a nonlinear Hamilton-Jacobi equation;

– the amplitude satisfies a linear transport equation, the coefficient of which is related to $\nabla_x\varphi$.

Notice that the main drawback of this method appears already at this level: we replace linear equations by nonlinear ones, loosing therefore the superposition principle.

The first, and crucial, problem to address is the notion of solution for both equations. A natural[1] framework concerning the Hamilton-Jacobi equation is the one of viscosity solutions, introduced independently by Kružkov [23, 24], and Crandall-Lions [11]. In this class, existence and uniqueness hold for the Cauchy problem, essentially in the class of Lipschitz continuous functions. The gradient of φ may therefore develop singularities in a finite time, and this causes the whole ansatz to break down since the energy of the wave (given by the square of its amplitude) concentrates on the shock lines. A natural alternative would be to seek for multivalued phases corresponding to crossing waves. Recently, several attempts have been made, see e.g. [3, 13–15, 21, 35, 41], but this leads to difficult problems from both viewpoints of theory and numerics. Notice that, apart from [15, 21], these approaches share the common feature to solve the eikonal equation using numerical tools which have been developed in the context of viscosity solutions. In particular, the multivalued algorithm proposed in [3, 4] roughly consists in splitting the computational domain in possibly overlapping zones called "big rays", in which the coupled system is to be solved.

We propose here a complete study of the corresponding system when the eikonal equation is solved in the viscosity sense. We prove existence and uniqueness results, as well as convergence theorems for relevant numerical methods. The context may seem limited, but the characterization of the

[1] at least from the point of view of stability!

solutions and the behaviour of the discretization are of full interest. Indeed, on the one hand, as we mentioned before, lots of numerical implementations are based on this framework. On the other hand, this viscosity solution corresponds to the phase of the first arriving wave, and is therefore useful in several applications (*e.g.* seismology [41]). Finally, even in this context, severe mathematical difficulties arise, essentially because the amplitude has to be sought in the class of measures. As we shall see in more detail below, the present state of the art concerning measure-valued solutions enforces us to stick to one-dimensional problems, which is of course a severe restriction. Two difficult questions remain open at this stage: first, how to deal with multi-valued solutions to the Hamilton-Jacobi equation; next, generalize to more realistic multi-dimensional situations. However, we shall show that the example of the two-dimensional Helmholtz equation may be rewritten in order to fall into this context.

Consequently, we plan to give precise mathematical results about exact solutions and numerical approximations of the following model problem:

$$\partial_t \varphi + \mathcal{H}(t, x, \partial_x \varphi) = 0, \tag{1}$$

$$\partial_t \mu + \partial_x (a\mu) = 0, \tag{2}$$

where the Hamiltonian $\mathcal{H}(t, x, p)$ is a smooth function, strictly convex in p, and a depends usually on the partial derivatives in space and time of φ. Therefore, both $\mathcal{H}$ and a may take different forms, and we shall give several explicit examples in Sect. 2: our results do not pretend to whole generality. Once we have chosen to solve (1) in the class of viscosity solutions, its x derivative is likely to blow up in finite time (for instance when caustics occur in geometrical optics) and the coefficient a may become discontinuous. In this case, μ is a measure in space; the precise meaning of a solution to (2), and in particular of the product $a\mu$, has to be explicited. There are very few attempts to consider this kind of problems. The approach used by Poupaud and Rascle [33] seems attractive here because it gives an existence result in the multidimensional case. The main drawback is that, so far, there are no stability results available, which is of course essential in proving convergence of numerical approximations. In this respect, a more appropriate notion, called *duality solutions*, was introduced in the one-dimensional case by Bouchut and James [5] (see also Petrova and Popov [32] for some extensions in the same context and [19]).

The key assumption to construct duality solutions is a one-sided Lipschitz condition (OSLC) on a, which ensures that the flow is somehow compressive. Under this restriction, existence, uniqueness of measure-valued solutions can be proved, as well as stability results with respect to perturbations of the coefficients. In the same context, the discretization of these solutions has been studied by the authors in [16], and involves a discrete analogue of the OSLC condition. Therefore, the first step in both theoretical and numerical studies of (1), (2) will be to obtain additional estimates on the viscosity solution φ.

The paper is organized as follows. In a first section, we present some examples where the system (1)-(2) naturally arises. Then, in the second one, we recall the definitions and some stability properties of viscosity and duality solutions, and state existence and uniqueness results for the coupled systems of the examples. Next, we study numerical approximations and give a convergence result towards the previously defined solutions. Both results mainly rely upon semiconcavity properties ensured by the eikonal equation, and by Lax-Friedrichs type schemes for its discretization. Finally, we illustrate the results with several numerical computations inspired by [20] for the Schrödinger equation, and [15, 37] for the Helmholtz equation.

2 Presentation of the examples

2.1 The 1D Schrödinger equation

In one space dimension, the Schrödinger equation reads

$$i\hbar\partial_t\Psi + \frac{\hbar^2}{2}\partial_{xx}\Psi = V(x)\Psi, \tag{3}$$

where V is the corresponding potential. A nonlinear version of this equation is obtained by replacing $V(x)$ by $U'(|\Psi|^2)$, where U is a real-valued smooth function. The parameter $\hbar$ is analogous to the Planck constant, and the semiclassical limit consists in considering initial data of the form

$$\Psi(0,x) = A^0(x)\exp\left(\frac{i}{\hbar}\varphi^0(x)\right), \qquad \hbar \to 0\ ,$$

where the amplitude $A^0 \geq 0$, and the real-valued phase φ^0 are smooth functions independant of $\hbar$. Inserting the ansatz

$$\Psi(t,x) = A(t,x)\exp\left(\frac{i}{\hbar}\varphi(t,x)\right) \tag{4}$$

in (3) yields after some easy formal computations an eikonal equation for φ, and a transport equation for A. More precisely, considering the coefficients of terms of order 0 in $\hbar$, we obtain

$$\partial_t\varphi + \frac{1}{2}(\partial_x\varphi)^2 + V = 0, \tag{5}$$

which can be rewritten as a Burgers equation with a source term by differentiating in x and setting $v = \partial_x \varphi$:

$$\partial_t v + \partial_x \left(\frac{v^2}{2} \right) + \partial_x V = 0. \tag{6}$$

Next, the order one terms lead to the following equation:

$$\partial_t A + v \partial_x A + \frac{1}{2} A \partial_x v = 0.$$

Multiplying this equation by $2A$ and setting $\mu = A^2$ leads to a linear conservation law for the energy:

$$\partial_t \mu + \partial_x (a\mu) = 0, \qquad \text{where} \quad a(t,x) = v(t,x) = \partial_x \varphi(t,x). \tag{7}$$

Therefore, considering the system constituted by the eikonal equation (5) and the conservation equation (7), we are exactly in the afore described context, with $\mathcal{H}(t,x,p) = p^2/2$ and $a = \partial_x \varphi$. Since $\partial_x \varphi$ is a solution to the Burgers equation, we know that discontinuities can develop in finite time, even starting from smooth initial data.

Notice that we can rewrite these equations in a different way, by introducing new variables $\rho = A^2$, and $q = A^2 v = \rho v$. This yields after a few straightforward computations

$$\partial_t \rho + \partial_x q = 0, \qquad \partial_t q + \partial_x (v\, q) + \rho \partial_x V = 0. \tag{8}$$

In particular, for $\partial_x V = 0$, *i.e.* for the free Schrödinger equation, we recover the pressureless gases system, which has been widely studied (see [7] for duality solutions, and the numerous references quoted there). These equations are usually interpreted as the macroscopic behaviour of the so-called sticky particles: when two particles collide, they stick together, forming a new particle. This interpretation fails obviously in the Schrödinger case, since the paths must cross each other here. When this occurs, the method breaks down, and actually, the unknown ρ becomes a measure in space.

2.2 The wave equation

The wave equation in an inhomogeneous medium endowed with a variable refraction index $\eta(x) > 0$, $x \in \mathbb{R}^d$, is

$$\partial_{tt} u - \frac{1}{\eta(x)^2} \Delta u = 0. \tag{9}$$

The light speed in the medium is $c(x) = 1/\eta(x)$ provided the velocity in the vacuum is normalized to 1. We are interested in highly oscillating solutions, with frquency $1/\varepsilon$, so we insert in (9) the same ansatz as for the Schrödinger equation: $u(t,x) = A(t,x)\exp(i\varphi(t,x)/\varepsilon)$. Once again, we perform an expansion in powers of ε. Annihilating the ε^{-2} term gives rise to the eikonal equation, while the ε^{-1} term leads to a linear transport equation for A. Notice that, if one wishes to compute higher order terms, the function A itself should be written as a power series in ε.

The eikonal equation reads here

$$(\partial_t\varphi)^2 - \frac{1}{\eta(x)^2}|\nabla\varphi|^2 = 0, \tag{10}$$

so that the Hamiltonian is $\mathcal{H}(t,x,p) = \pm p/\eta(x)$. In its whole generality, the transport equation is given by (∂_j stands here for $\frac{\partial}{\partial x_j}$)

$$\partial_t\varphi\partial_t A - \frac{1}{\eta(x)^2}\sum_{j=1}^{d}\partial_j\varphi\partial_j A + \frac{1}{2}\left(\partial_{tt}\varphi - \frac{1}{\eta(x)^2}\Delta\varphi\right)A = 0. \tag{11}$$

We shall be interested in two simple cases, namely $d = 1$ and radial solutions, where η, u, A and φ depend only on $r = |x|$.

In the one-dimensional case, the eikonal equation reduces to the pair of linear equations $\partial_t\varphi \pm \frac{1}{\eta(x)}\partial_x\varphi = 0$. This readily gives the expression of the time derivative of φ in terms of the space derivative. Plugging these results into the transport equation (11) leads to

$$\partial_t A \pm \frac{1}{\eta}\partial_x A - \frac{A}{2}\partial_x\left(\frac{1}{\eta}\right) = 0. \tag{12}$$

For both choices of the sign, this equation can be rewritten in a conservative form. Namely, for the minus sign, we multiply by $2A$ to obtain the conservation of the energy A^2, and for the plus sign, we get the conservation of $1/A^2$ by multiplying by $-2/A^3$. Once again, we recover a system in the form (1)-(2), with

- $\mathcal{H}(t,x,p) = p/\eta(x)$, $a(t,x) = 1/\eta(x)$ and $\mu = 1/A^2$ for the plus sign;
- $\mathcal{H}(t,x,p) = -p/\eta(x)$, $a(t,x) = -1/\eta(x)$ and $\mu = A^2$ for the minus sign.

In this particular case, provided η is a smooth function, the conservation equation we obtain has a smooth coefficient, so that no singularities appear. The notion of duality solutions allows to consider nonsmooth η's. For instance, considering $\mathcal{H}(t,x,p) = -p/\eta(x)$, $\mu = A^2$, and $a(t,x) = -1/\eta(x)$, if η is only assumed to be bounded and one- sided Lipschitz continuous, the results in [6,16] apply, so that

- there exists a unique pair of duality solutions (φ,μ) of the differential Cauchy problem;

- a broad class of conservative numerical schemes converge to these weak solutions under some explicit CFL restrictions.

For $d > 1$, and radial behaviour, the computations are almost identical, and make use of the equality $\Delta_x u(|x|) = \partial_{rr} u - \frac{d-1}{r}\partial_r u$. The eikonal equation boils down to the pair $\partial_t \varphi \pm \frac{1}{\eta(r)}\partial_r \varphi = 0$, and the transport equation is here

$$\partial_t A \pm \partial_r A + \frac{1}{2}\left(-\partial_r \frac{1}{\eta} \pm \frac{1}{\eta}\frac{d-1}{r}\right) = 0.$$

Once again, we can obtain two conservation laws from this equation. For the plus sign, we multiply by $-2/(r^{d-1}a^3)$ to get

$$\partial_t \left(\frac{1}{r^{d-1}a^2}\right) + \partial_r \left(\frac{1}{\eta r^{d-1}a^2}\right) = 0,$$

and for the minus sign, multiplying by $2r^{d-1}a$ leads to

$$\partial_t \left(r^{d-1}a^2\right) - \partial_r \left(\frac{1}{\eta} r^{d-1}a^2\right) = 0.$$

In the case where the refraction index $\eta(x)$ is smooth, no measure-valued solutions occur as for $d = 1$. However, there is a geometrical singularity, which is clearly evidenced even for a constant η. Indeed in this case, the transport equation shows that the quantity $r^{d-1}a^2$ is conserved inside ray tubes, and therefore the energy A^2 diverges like $1/r^{d-1}$ at the origin.

2.3 The 2D Helmholtz equation

If one looks for planar wave solutions $\tilde{u}(t, \mathbf{x}) = u(\mathbf{x})\exp(ikt)$ to the wave equation (9), one is led to find a steady function u satisfying the scalar Helmholtz equation:

(13) $$\Delta u + k^2\,\eta^2\,u = 0,$$

We shall consider here the two-dimensional equation, and set $\mathbf{x} = (x_1, x_2)$. Searching for solutions oscillating with frequency k, it is natural to use the same kind of ansatz as previously, namely $u(x_1, x_2) = A(x_1, x_2)$ $\exp(ik\varphi(x_1, x_2))$. Cancelling the first two terms in the power expansion in k leads to the following stationary system:

(14) $$|\nabla\varphi| = \eta, \qquad 2\,\nabla A \cdot \nabla\varphi + A\Delta\varphi = 0.$$

We refer the reader to e.g. [1,22,29,34,45] for details on this derivation. The stationary transport equation for A leads to a linear conservation law for the energy A^2:

(15) $$\nabla \cdot (A^2 \nabla\varphi) = 0.$$

We aim at rewriting this system in such a way that it matches the previously defined context, in order to apply the aforementioned theoretical results we are about to prove. An important obstruction to treat (14) as it stands is indeed the handling of a boundary-value problem within a class of measure-valued solutions. One alternative is then to select a privileged direction of propagation in (14), say x_2, and to consider it as a "time– like" direction. This paraxial-type assumption compels us to assume $\partial_{x_2}\varphi > 0$ in the domain of interest, but this is of common use in several applications including seismology (cf e.g. [41]) or computations of lenses. Therefore, we rewrite the eikonal equation the following way:

$$\partial_{x_2}\varphi - \sqrt{\eta^2 - (\partial_{x_1}\varphi)^2} = 0$$

Then, it is meaningful to introduce a quantity $\mu = A^2.\partial_{x_2}\varphi$ and the conservation equation (15) rewrites:

$$\partial_{x_2}\mu + \partial_{x_1}\left(\mu\,\frac{\partial_{x_1}\varphi}{\partial_{x_2}\varphi}\right) = 0.$$

We are once again in the general context if we set as a "time" variable $t = x_2$ and as a "space" one $x = x_1$: this leads to $\mathcal{H}(t,x,p) = -\sqrt{\eta^2(t,x) - p^2}$ and $a(t,x) = \frac{\partial_x\varphi(t,x)}{\partial_t\varphi(t,x)}$. Notice that, in contrast with the wave equation, the Hamiltonian depends on the "time" variable.

3 Weak solutions to the differential problem

3.1 An appropriate notion of solutions

The resolution of the Cauchy problem (1)-(2) we have in mind involves two different notions of solutions: viscosity solutions for the inhomogeneous eikonal equation and duality solutions for the linear conservation equation.

For the reader's convenience, we recall here both definitions, as well as basic results which are to be used in the sequel. We begin with viscosity solutions, which were introduced under that name by Crandall and Lions, [11], see also Kružkov's papers [23, 24].

Definition 1 *Let $\mathcal{H} \in C([0,T]\times\mathbb{R}\times\mathbb{R})$. A function $\varphi \in C(]0,T]\times\mathbb{R})$ is a* **viscosity solution** *of (1) if for every $\chi \in C^\infty(]0,T]\times\mathbb{R})$, there holds:*

- *if $(\varphi-\chi)$ has a local maximum point at $(t_0,x_0)\in]0,T[\times\mathbb{R}$, then:*

$$\partial_t\chi(t_0,x_0) + \mathcal{H}(t_0,x_0,\partial_x\chi(t_0,x_0)) \le 0;$$

- *if $(\varphi-\chi)$ has a local minimum point at $(t_0,x_0)\in]0,T[\times\mathbb{R}$, then*

$$\partial_t\chi(t_0,x_0) + \mathcal{H}(t_0,x_0,\partial_x\chi(t_0,x_0)) \ge 0.$$

If moreover, $\varphi \in C([0,T] \times \mathbb{R})$ *and* $\varphi(0,x) = \varphi^0(x)$*, an initial datum prescribed for* $x \in \mathbb{R}$*, then* φ *is a viscosity solution on* $[0,T] \times \mathbb{R}$.

We summarize here several existence and regularity results for viscosity solutions. Proofs, more detailed and precise results are to be found in [2,10, 11,39,40].

Theorem 1 *Assume that the Hamiltonian* $\mathcal{H}$ *in (1) satisfies:*

(i) $\mathcal{H}$ *is uniformly continuous on* $[0,T] \times \mathbb{R} \times [-R,R]$ *for all* $R > 0$*;*
(ii) $\sup_{[0,T]\times\mathbb{R}} |\mathcal{H}(t,x,0)| \equiv M < +\infty$;
(iii) There exists a constant $C > 0$ *such that, for all* $t \in [0,T]$*,* $x, y, p \in \mathbb{R}$*,*

$$|\mathcal{H}(t,x,p) - \mathcal{H}(t,y,p)| \leq C\,(1 + |p|)\,|x - y|$$

Consider $\varphi(0,.) = \varphi^0 \in$ *Lip* $\cap\, BUC(\mathbb{R})$*: there exists a unique viscosity solution* $\varphi \in BUC([0,T] \times \mathbb{R})$*, which belongs to Lip*$([0,T] \times \mathbb{R})$.

Remark 1. Actually, we have for any $0 \leq t \leq T$

(16) $$\mathrm{Lip}(\varphi(t,.)) \leq \mathrm{Lip}(\varphi^0) + Ct\Big(1 + \sup_{0\leq\tau\leq T} \mathrm{Lip}(\varphi(\tau,.))\Big).$$

We now turn to the notion of duality solutions, which were introduced by Bouchut and James in [5,6] to solve in the context of measures the linear conservation equation (2) when the discontinuous coefficient a is L^∞ bounded and satisfies the one-sided Lipschitz condition (OSLC)

(17) $$\partial_x a \leq \alpha, \qquad \text{with} \quad \alpha \in L^1(]0,T[).$$

Recall that duality solutions are defined as weak solutions, the test functions being Lipschitz solutions to the backward linear transport equation

(18) $$\partial_t p + a(t,x)\partial_x p = 0, \quad p(T,.) = p^{\mathrm{T}} \in \mathrm{Lip}(\mathbb{R}).$$

A formal computation shows that $\partial_t(p\mu) + \partial_x[a(t,x)p\mu] = 0$, and thus

(19) $$\frac{d}{dt}\left(\int_{\mathbb{R}} p(t,x)\mu(t,dx)\right) = 0,$$

which defines the duality solutions for suitable p's. It is quite classical that (17) ensures existence for (18), but not uniqueness, which is of great importance here to obtain stability results. However, existence of solutions to (18) was already used in the context of nonlinear conservation laws, to obtain uniqueness of solutions (see Oleinik [31]), or error estimates (see Tadmor [44]).

Therefore, the corner stone in the construction of duality solutions is the introduction of the notion of *reversible* solutions to (18). A complete statement of the definitions and properties of reversible solutions would be too long in the present context, so that merely a few hints are given. Let $\mathcal{L}$ denote the set of Lipschitz continuous solutions to (18), and define the set of *exceptional solutions*:

$$\mathcal{E} = \Big\{ p \in \mathcal{L} \text{ such that } p^{\mathrm{T}} \equiv 0 \Big\}.$$

The possible loss of uniqueness corresponds to the case where $\mathcal{E}$ is not reduced to zero.

Definition 2 *We say that $p \in \mathcal{L}$ is a* **reversible solution** *to (18) if p is locally constant on the set*

$$\mathcal{V}_e = \Big\{ (t,x) \in [0,T] \times \mathbb{R};\ \exists\, p_e \in \mathcal{E},\ p_e(t,x) \neq 0 \Big\}.$$

Consider the example $a(x) = -\operatorname{sgn}(x)$. Then we have $\mathcal{V}_e = \{(t,x) \in [0,T] \times \mathbb{R};\ |x| < T - t\}$, the solution is defined by the characteristics outside $\mathcal{V}_e$, and we choose to prescribe $p(t,x) = p^{\mathrm{T}}(0)$ inside $\mathcal{V}_e$.

This definition leads quite directly to the uniqueness results of [5,6]. It turns out that the class of reversible solutions is also stable by perturbations of the coefficient a, in a sense precisely stated in Theorem 2 below. The proof of this result makes use of more handable characterizations of reversible solutions, involving especially monotonicity, but we shall not need here these precise statements.

Theorem 2 *(Bouchut, James [5,6])*
1) Let $p^{\mathrm{T}} \in Lip_{loc}(\mathbb{R})$. Then there exists a unique $p \in \mathcal{L}$ reversible solution to (18) such that $p(T,.) = p^{\mathrm{T}}$.
2) Let (a_n) be a bounded sequence in $L^\infty([0,T] \times \mathbb{R})$, with $a_n \rightharpoonup a$ in $L^\infty([0,T] \times \mathbb{R}) - w\star$. Assume $\partial_x a_n \leq \alpha_n(t)$, where (α_n) is bounded in $L^1(]0,T[)$, $\partial_x a \leq \alpha \in L^1(]0,T[)$. Let (p_n^{T}) be a bounded sequence in $Lip_{loc}(\mathbb{R})$, $p_n^{\mathrm{T}} \to p^{\mathrm{T}}$, and denote by p_n the reversible solution to

$$\partial_t p_n + a_n \partial_x p_n = 0 \quad \text{in }]0,T[\times\mathbb{R}, \qquad p_n(T,.) = p_n^{\mathrm{T}}.$$

Then $p_n \to p$ in $C([0,T] \times [-R,R])$ for any $R > 0$, where p is the reversible solution to

$$\partial_t p + a \partial_x p = 0 \quad \text{in }]0,T[\times\mathbb{R}, \qquad p(T,.) = p^{\mathrm{T}}.$$

We now restrict ourselves to those p's in (19): more precisely, we state the following definition.

Definition 3 *We say that* $\mu \in \mathcal{S}_{\mathcal{M}} \equiv C([0,T];\mathcal{M}_{loc}(\mathbb{R}) - \sigma(\mathcal{M}_{loc}, C_c))$ *is a* **duality solution** *to (2) if for any* $0 < \tau \leq T$*, and any* **reversible** *solution* p *to (18) with compact support in* x*, the function* $t \mapsto \int_{\mathbb{R}} p(t,x)\mu(t,dx)$ *is constant on* $[0,\tau]$.

We shall need the following facts concerning duality solutions.

Theorem 3 *(Bouchut, James [5,6])*
1) Given $\mu^\circ \in \mathcal{M}_{loc}(\mathbb{R})$*, under the assumptions (17), there exists a unique* $\mu \in \mathcal{S}_{\mathcal{M}}$*, duality solution to (2), such that* $\mu(0,.) = \mu^\circ$.
2) There exists a bounded Borel function $\widehat{a}$*, called* **universal representative** *of* a*, such that* $\widehat{a} = a$ *almost everywhere, and for any duality solution* μ*,*

$$\partial_t \mu + \partial_x(\widehat{a}\mu) = 0 \qquad \textit{in the distributional sense.}$$

3) Let (a_n) *be a bounded sequence in* $L^\infty(]0,T[\times\mathbb{R})$*, such that* $a_n \rightharpoonup a$ *in* $L^\infty(]0,T[\times\mathbb{R}) - w\star$*. Assume* $\partial_x a_n \leq \alpha_n(t)$*, where* (α_n) *is bounded in* $L^1(]0,T[)$*,* $\partial_x a \leq \alpha \in L^1(]0,T[)$*. Consider a sequence* $(\mu_n) \in \mathcal{S}_{\mathcal{M}}$ *of duality solutions to*

$$\partial_t \mu_n + \partial_x(a_n \mu_n) = 0 \quad \textit{in} \quad]0,T[\times\mathbb{R},$$

such that $\mu_n(0,.)$ *is bounded in* $\mathcal{M}_{loc}(\mathbb{R})$*, and* $\mu_n(0,.) \rightharpoonup \mu^\circ \in \mathcal{M}_{loc}(\mathbb{R})$*. Then* $\mu_n \to \mu$ *in* $\mathcal{S}_{\mathcal{M}}$*, where* $\mu \in \mathcal{S}_{\mathcal{M}}$ *is the duality solution to*

$$\partial_t \mu + \partial_x(a\mu) = 0 \quad \textit{in} \quad]0,T[\times\mathbb{R}, \qquad \mu(0,.) = \mu^\circ.$$

Moreover, $\widehat{a}_n \mu_n \rightharpoonup \widehat{a}\mu$ *weakly in* $\mathcal{M}_{loc}(]0,T[\times\mathbb{R})$.

The set of duality solutions is clearly a vector space, but it has to be noted that a duality solution is not *a priori* defined as a solution in the sense of distributions. The product $\widehat{a}\mu$ is defined *a posteriori*, by the equation itself (see assertion 2 in the above theorem).

3.2 Existence and uniqueness results

In this paragraph, we turn to the Cauchy problem associated to (1)-(2): take any pair of initial data $(\mu^0, \varphi^0) \in \mathcal{M}(\mathbb{R}) \times W^{1,\infty}(\mathbb{R})$, such that a semiconcavity estimate holds for some $\gamma \in \mathbb{R}^+$,

$$\max(0, \partial_{xx}\varphi^0) \leq \gamma < +\infty, \tag{20}$$

and consider

$$\begin{cases} \partial_t \varphi + \mathcal{H}(t,x,\partial_x \varphi) = 0 \\ \partial_t \mu + \partial_x(a(t,x)\mu) = 0 \end{cases} \text{in }]0,T[\times\mathbb{R}, \qquad \begin{cases} \varphi(0,.) = \varphi^0 \\ \mu(0,.) = \mu^0 \end{cases}. \tag{21}$$

We wish to give additional conditions on the parameters in order to ensure the existence and uniqueness of a pair of viscosity/duality solutions to (21) in the context of the examples presented in the previous section. The proof consists essentially in three steps:

– to establish existence and uniqueness for the viscosity solution of the Hamilton-Jacobi equation;
– to ensure that a semiconcavity estimate of the form (20) holds true for any $t > 0$;
– to prove that this semiconcavity implies the OSLC condition on a, which gives existence and uniqueness of the duality solution to the conservation equation.

The key point here is of course the second one, and it is worth giving here a general lemma.

Lemma 1 *Consider a Hamiltonian $\mathcal{H}$ satisfying the assumptions of Theorem 1, and an initial datum $\varphi^0 \in W^{1,\infty}(\mathbb{R})$ such that (20) holds true. Assume in addition $\mathcal{H}$ of class C^2, with*

$$\partial_{pp}\mathcal{H} \geq \zeta_0 > 0, \tag{22}$$

and, for all $R > 0$,

$$\begin{aligned} \inf_{(t,x,p)\in[0,T]\times\mathbb{R}\times[-R,R]} \partial_{xp}\mathcal{H}(t,x,p) > -\infty, \\ \inf_{(t,x,p)\in[0,T]\times\mathbb{R}\times[-R,R]} \partial_{xx}\mathcal{H}(t,x,p) > -\infty. \end{aligned} \tag{23}$$

Then the viscosity solution φ satisfies the following semiconcavity estimate:

$$\forall t \in [0,T], \quad \max(0, \partial_{xx}\varphi(t,.)) \leq \max(\Gamma, \gamma) < +\infty, \tag{24}$$

where Γ is a constant depending on $\mathcal{H}$, and γ is defined by (20).

Remark 2. Such kind of semiconcavity estimates already exist in the literature, for Hamiltonians convex in the p variable, see e.g. Kružkov [23], or Lions [28]. We deal here with Hamiltonians depending also upon the time and space variables. This was indicated by Lin and Tadmor [27], even for multidimensional Hamiltonians, but with a convexity assumption in x, which we drop here.

Proof of Lemma 1. It is known that existence and uniqueness hold for smooth viscosity solutions to the regularized equation $\partial_t\varphi^\varepsilon + \mathcal{H}(t,x,\partial_x\varphi^\varepsilon) = \varepsilon\partial_{xx}\varphi^\varepsilon$, and that φ^ε converges towards the viscosity solution φ to (1) when ε goes to zero (see e.g. [39]). Therefore we need to prove the above estimate uniformly in ε for φ^ε. Differentiating twice the viscous equation with respect to x and setting $z = \partial_{xx}\varphi^\varepsilon$ leads to:

$$\begin{aligned}&\partial_t z + \partial_{pp}\mathcal{H}(t,x,\partial_x\varphi^\varepsilon)z^2 + 2\partial_{xp}\mathcal{H}(t,x,\partial_x\varphi^\varepsilon)z + \\ &\partial_{xx}\mathcal{H}(t,x,\partial_x\varphi^\varepsilon) + \partial_p\mathcal{H}(t,x,\partial_x\varphi^\varepsilon)\partial_x z = \varepsilon\partial_{xx}z.\end{aligned}$$

From (16), we deduce that, for some constant M depending only upon the initial datum φ^0 and T, there holds $\|\partial_x\varphi^\varepsilon\|_\infty \le M$. By (23), the quantities

$$\begin{aligned}\zeta_1 &= \min\Big(0, \inf_{(t,x)\in[0,T]\times\mathbb{R};|p|\le M} \partial_{xp}\mathcal{H}(t,x,p)\Big),\\ \zeta_2 &= \min\Big(0, \inf_{(t,x)\in[0,T]\times\mathbb{R};|p|\le M} \partial_{xx}\mathcal{H}(t,x,p)\Big),\end{aligned} \tag{25}$$

are well-defined and nonpositive. Hence, $z^+ = \max(0, \partial_{xx}\varphi^\varepsilon)$ satisfies:

$$\partial_t z^+ + \zeta_0(z^+)^2 + 2\zeta_1 z^+ + \zeta_2 + \partial_p\mathcal{H}(t,x,\partial_x\varphi^\varepsilon)\partial_x z^+ \le \varepsilon\partial_{xx}z^+,$$

and $\bar{z}^+(t) \stackrel{\text{def}}{=} \sup_{x\in\mathbb{R}} z^+(t,x)$ is a subsolution to the following Ricatti differential equation:

$$\frac{d}{dt}\bar{z}^+ + \zeta_0(\bar{z}^+)^2 + 2\zeta_1\bar{z}^+ + \zeta_2 = 0.$$

Since $\zeta_0 > 0$ and $\zeta_1, \zeta_2 \le 0$, the roots of $\zeta_0 X^2 + \zeta_1 X + \zeta_2$ are real, and we denote by Γ the largest one. Therefore we get immediately $\bar{z}^+(t) \le \max(\bar{z}^+(0), \Gamma)$, and we are done. □

Remark 3. As a consequence of this proof, following again [27], one can obtain a convergence rate of φ^ε towards φ, provided the initial data are in $L^1(\mathbb{R})$. More precisely, we have: $\|\varphi^\varepsilon(t,.) - \varphi(t,.)\|_{L^1(\mathbb{R})} = C(T)\varepsilon$ for all $0 \le t \le T$.

Notice that this lemma does not apply to the Hamiltonian of the wave equation, since then $\partial_{pp}\mathcal{H} \equiv 0$. But in this last case, the eikonal equation is therefore a linear transport equation, so that the semiconcavity of the solution is the same as the one of the initial data. We turn now to specific results for our examples.

Theorem 4 *(The Schrödinger case) Under the semiconcavity requirement (20) on $\varphi^0 \in W^{1,\infty}(\mathbb{R})$, there exists a unique couple of viscosity/duality solutions to the Cauchy problem (21).*

Proof. Here $\mathcal{H}(t,x,p) = p^2/2$ satisfies all the requirements of Theorem 1 and Lemma 1. Hence there exists a unique viscosity solution to (1), and the semiconcavity propagates. Since $a = \partial_x\varphi$, this means exactly that we have the OSLC property, so that existence and uniqueness hold in the duality sense for (2). □

The analogous result for the Helmholtz equation is slightly more difficult, since the Hamiltonian $\mathcal{H}(t,x,p) = -\sqrt{\eta^2(t,x) - p^2}$ is not uniformly continuous. The final result is:

Theorem 5 *(The Helmholtz equation)*
Consider $\eta \in C^2 \cap W^{2,\infty}([0,T] \times \mathbb{R})$, with $0 < \eta_0 \leq \eta$ and $\partial_t \eta \geq 0$. Assume $\varphi^0 \in W^{1,\infty}(\mathbb{R})$ satisfies (20) and, for all $x \in \mathbb{R}$,

$$\Big(\eta(0,x)\Big)^2 - \Big(\partial_x \varphi^0(x \pm 0)\Big)^2 \geq \beta^2 > 0. \tag{26}$$

Then there exists a unique couple of viscosity/duality solutions of the Cauchy problem (21).

We begin by a lemma ensuring existence and uniqueness of the viscosity solution. The corner stone is actually to prove that (26) propagates for all $t > 0$, so that $\mathcal{H}$ remains uniformly continuous on the domain of values of the solution.

Lemma 2 *Consider $0 \leq \eta \in C^2 \cap W^{2,\infty}([0,T] \times \mathbb{R})$, with $\partial_t \eta \geq 0$, and let $\varphi^0 \in W^{1,\infty}(\mathbb{R})$ satisfy (26) for all $x \in \mathbb{R}$. Then there exists a unique viscosity solution $\varphi \in W^{1,\infty}([0,T] \times \mathbb{R})$ to the Cauchy problem corresponding to (1) with initial data φ^0.*

Proof. The key point is to get sufficient conditions to ensure that there exists a solution φ to (1) such that $\eta^2 - (\partial_x \varphi)^2$ is always positive. Once this is done, we know by Theorem 1 that it is the viscosity solution, because the Hamiltonian is uniformly continuous on the domain $\eta^2 - p^2 \geq \beta^2 > 0$. We proceed by approximation, and consider the equation

$$\partial_t \varphi_\varepsilon + \mathcal{H}_\varepsilon(t,x,\partial_x \varphi_\varepsilon) = \varepsilon \partial_{xx} \varphi_\varepsilon, \tag{27}$$

where the approximate Hamiltonian $\mathcal{H}_\varepsilon(t,x,p)$ is defined in the following way. We pick up a convex function Ψ_ε which satisfies for $\varepsilon > 0$:

$$\Psi_\varepsilon \in C^\infty(\mathbb{R}), \quad \Psi_\varepsilon(0) = \varepsilon/2, \quad \Psi_\varepsilon(x) = |x| \text{ for } |x| \geq \varepsilon.$$

Convexity implies that $|(\Psi_\varepsilon)'| \leq 1$. Then we define $\mathcal{H}_\varepsilon(t,x,p) = -\sqrt{\Psi_\varepsilon(\eta^2(t,x) - p^2)}$. The classical theory of parabolic equations ensures that there exists a unique solution to (27), and that it is the viscosity solution (see e.g. [39]). Indeed, $\mathcal{H}_\varepsilon$ is uniformly continuous on $[0,T] \times \mathbb{R} \times \mathbb{R}$ and $\sup_{(t,x)\in[0,T]\times\mathbb{R}} |\mathcal{H}_\varepsilon(t,x,0)| = \|\eta\|_\infty$, so that the first two requirements of Theorem 1 are satisfied. Using Taylor expansions, we see that in the last requirement, we can choose $C = \|\eta\|_\infty \cdot \|\partial_x \eta\|_\infty / \sqrt{\varepsilon}$. Therefore we have to ensure that under appropriate restrictions on the initial data and the refraction index, we always have $\bar{w}(t) \stackrel{\text{def}}{=} \sup_{x\in\mathbb{R}} \Big[(\partial_x \varphi_\varepsilon)^2(t,x) - \eta^2(t,x)\Big] \leq$

$-\varepsilon_0 < 0$ for all $t \in [0, T]$. So, denoting $v = \partial_x \varphi_\varepsilon$, $w = \frac{1}{2}(v^2 - \eta^2)$, we differentiate (27) with respect to x. We get a viscous conservation law:

$$\partial_t v - \partial_x \Big(\sqrt{\Psi_\varepsilon(\eta^2(t,x) - v^2)} \Big) = \varepsilon \partial_{xx} v.$$

Since v is smooth enough, we can apply the chain rule:

$$\partial_t v - \frac{(\eta \cdot \partial_x \eta - v \cdot \partial_x v) \Psi'_\varepsilon(\eta^2 - v^2)}{\sqrt{\Psi_\varepsilon(\eta^2 - v^2)}} = \varepsilon \partial_{xx} v.$$

We notice that $\partial_t w = v \cdot \partial_t v - \eta \cdot \partial_t \eta$, $\partial_x w = v \cdot \partial_x v - \eta \cdot \partial_x \eta$, and $\partial_{xx} w = (\partial_x v)^2 + v \cdot \partial_{xx} v - (\partial_x \eta)^2 - \eta \cdot \partial_{xx} \eta$. So, multiplying by v and inserting these values leads to:

$$\partial_t w + \partial_t \eta \cdot \eta - v \cdot \partial_x w \cdot \frac{\Psi'_\varepsilon(\eta^2 - v^2)}{\sqrt{\Psi_\varepsilon(\eta^2 - v^2)}}$$
$$= \varepsilon \Big\{ \partial_{xx} w - (\partial_x v)^2 + (\partial_x \eta)^2 + \eta \cdot \partial_{xx} \eta \Big\}$$

The quantity $\bar{w}(t)$ therefore evolves according to:

$$\text{(28)} \qquad \frac{d}{dt}\bar{w} - \varepsilon \inf_{x \in \mathbb{R}} \Big((\partial_x \eta)^2 + \eta \cdot \partial_{xx} \eta \Big) \leq - \inf_{x \in \mathbb{R}} (\eta \cdot \partial_t \eta).$$

Taking into account both the $W^{2,\infty}$ norm of η and the sign of $\partial_t \eta$ gives us the required uniform in ε bound on the x-derivative of φ_ε. This bound passes to the limit $\varepsilon \to 0$, so we are done. □

Remark 4. The sign assumption on $\partial_t \eta$ ensures that $\bar{w}$ is a nonincreasing function of time (see (28) in the above proof). It is therefore possible to weaken it when T is small enough and the initial datum induces a large enough β^2.

Proof of Theorem 5. From Lemma 2, we have existence and uniqueness of the viscosity solution to (1). In order to prove the existence of the duality solution to (2), we only have to check that the coefficient $a = \partial_x \varphi / \partial_t \varphi$ satisfies the L^∞ and OSLC bounds. We have $a = \frac{\partial_x \varphi}{\sqrt{\eta^2 - (\partial_x \varphi)^2}} \in L^\infty([0,T] \times \mathbb{R})$ as a simple consequence of Lemma 2. Next, we observe that

$$\partial_x a = \frac{\eta^2 \cdot \partial_{xx} \varphi}{(\eta^2 - (\partial_x \varphi)^2)^{\frac{3}{2}}},$$

so that a satisfies (17) as soon as φ is semiconcave. We just need to check that $\mathcal{H}$ satisfies the assumptions of Lemma 1. But $\partial_{pp}\mathcal{H}(t,x,p) = \frac{\eta^2}{(\eta^2 - p^2)^{\frac{3}{2}}} \geq \frac{\eta_0^2}{(2\|\eta\|_\infty)^{\frac{3}{2}}} \equiv \zeta_0 > 0$, and the quantities ζ_1, ζ_2 defined in (23) are well-defined by the assumptions on η. Therefore, $\varphi(t,.)$ is semiconcave for all $t > 0$, which allows us to conclude. □

Remark 5. The assumption $\eta \in C^2 \cap W^{2,\infty}([0,T]\times\mathbb{R})$ may seem restrictive, but it is actually required to define φ as a local minimum in the Fermat principle according to e.g. [3].

4 Convergence of numerical approximations

Starting from here, we introduce a uniform grid defined by the two positive parameters Δx and Δt denoting respectively the mesh-size and the time-step. We shall denote, for $(j,n) \in \mathbb{Z}\times\mathbb{N}$, $x_j = j\Delta x$, $x_{j+1/2} = (j+1/2)\Delta x$, $t^n = n\Delta t$, and

$$T_j^n = \left[t^n, t^{n+1}\right[\times \left[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}\right[.$$

As usual, the parameter λ will refer to $\Delta t/\Delta x$, and we shall write for short $\Delta \to 0$ when $\Delta t, \Delta x \to 0$ with a fixed λ.

4.1 Lax-Friedrichs type schemes for the eikonal equation

In this section, we want to derive a first set of properties satisfied by the numerical approximations generated by three-point Lax-Friedrichs type schemes on the problem (1). This class of (simple) schemes has been studied in the context of Hamilton-Jacobi equations in e.g. [12,40]. We essentially refer to [40] for all the precise convergence results and error estimates.

In this work, we consider a slight variant of the Lax-Friedrichs scheme proposed in [12] by defining our numerical Hamiltonian as follows:

$$\mathsf{H}^{LF}(t,x,p^-,p^+) = \frac{1}{2}\left[\mathcal{H}(t,x,p^-) + \mathcal{H}(t,x,p^+) - \frac{\theta}{\lambda}(p^+ - p^-)\right]; \tag{29}$$

with $0 < \theta \leq 1$. This class of numerical schemes reads

$$\varphi_j^{n+1} = \varphi_j^n - \Delta t \mathsf{H}^{LF}\left(t^n, x_j, \frac{\varphi_j^n - \varphi_{j-1}^n}{\Delta x}, \frac{\varphi_{j+1}^n - \varphi_j^n}{\Delta x}\right), \tag{30}$$

and we introduce the piecewise constant function φ^Δ defined by

$$\varphi^\Delta(t,x) = \varphi_j^n \quad \text{for } (t,x) \in T_j^n.$$

We assume also that the discretization of the initial data has been properly chosen, in order that

$$\varphi^\Delta(0,.) \to \varphi^0 \text{ as } \Delta x \to 0,$$

strongly in $L^\infty(\mathbb{R})$. This can be achieved by defining each φ_j^0 as the pointwise value $\varphi^0(x_j)$ or the local average of φ^0 on $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}[$.

The coefficient θ introduces some artificial viscosity in the scheme. For $\theta = 0$, we get the centered scheme, which is unstable, for $\theta = 1$ the standard viscosity of the classical Lax-Friedrichs scheme. For $\theta > 1$, spurious oscillations develop.

The so-called consistency property, *i.e.* $\mathsf{H}^{LF}(t,x,p,p) = \mathcal{H}(t,x,p)$, is obviously satisfied. Next, introducing the same notations as in [12], we set

$$\varphi_j^n = G(t^n, x_j, \varphi_{j-1}^n, \varphi_j^n, \varphi_{j+1}^n),$$

where $G(t,x,\varphi_{-1},\varphi_0,\varphi_{+1}) = \varphi_0 - \Delta t \mathsf{H}^{LF}\Big(t, x, \dfrac{\varphi_0-\varphi_{-1}}{\Delta x}, \dfrac{\varphi_{+1}-\varphi_0}{\Delta x}\Big)$.

We denote $\mathbf{p} = (p^-, p^+) \in \mathbb{R}^2$. According to [40], the following regularity properties on the numerical Hamiltonian are needed:

- H^{LF} is uniformly continuous on $[0,T] \times \mathbb{R} \times [-R,R]^2$, for all $R > 0$;
- $\sup_{(t,x)\in[0,T]\times\mathbb{R}} |\mathsf{H}^{LF}(t,x,0,0)| \le K$ for some $K > 0$;
- there exists $C > 0$ such that, for all $s,t \in [0,T]$, $x,y \in \mathbb{R}$, $\mathbf{p} \in \mathbb{R}^2$, $|\mathsf{H}^{LF}(t,x,\mathbf{p}) - \mathsf{H}^{LF}(s,y,\mathbf{p})| \le C(1+|\mathbf{p}|)(|t-s|+|x-y|)$;
- there exists $M > 0$ such that, for all $t \in [0,T]$, $x \in \mathbb{R}$, $\mathbf{p_1}, \mathbf{p_2} \in (\mathbb{R}^2)^2$ with $|\mathbf{p_1}|, |\mathbf{p_2}| \le R$, $\quad |\mathsf{H}^{LF}(t,x,\mathbf{p_1}) - \mathsf{H}^{LF}(t,x,\mathbf{p_2})| \le M|\mathbf{p_1}-\mathbf{p_2}|$.

Provided $\mathcal{H}$ is C^1 in all the variables, most of these properties are obviously satisfied. Actually, exactly as in the continuous case, we shall have no problem with the Schrödinger equation, and need some technicalities for the Helmholtz equation.

The same way, the last important property, namely monotonicity, will be easy to check by differentiation as soon as we have enough regularity on $\mathcal{H}$, since we want G to be nondecreasing in each of the variables $\varphi_{-1}, \varphi_0, \varphi_{+1}$. Simple computations lead to the following statement (see [12,40]): the scheme (29)- (30) is monotone for $p \in [-R,R]$ under the CFL condition

$$\lambda \sup_{\substack{(t,x)\in\mathbb{R}\times[0,T] \\ |p|\le R}} |\partial_p \mathcal{H}(t,x,p)| \le \theta \le \frac{1}{2}. \tag{31}$$

Concerning the 1-d Schrödinger equation, the following result can be directly derived by estimating R in (31), since in this case, we have $\mathcal{H}(t,x,p) = p^2/2$.

Theorem 6 *(numerical convergence for the Schrödinger equation) The function φ^Δ generated by the Lax-Friedrichs type scheme (29)-(30) converges in $L^\infty([0,T]\times\mathbb{R})$ towards the viscosity solution of (1) under the CFL condition: $\lambda\Big(Lip(\varphi^0) + T\cdot Lip(\eta)\Big) \le \theta \le \frac{1}{2}$.*

Concerning the Helmholtz equation, we have the same kind of technical restriction on the refraction index as in the continuous case. Therefore we state the following theorem.

Theorem 7 *Under the assumptions of Theorem 5, the sequence of numerical approximations φ^Δ generated by the scheme (29)-(30) converges in $L^\infty([0,T]\times\mathbb{R})$ towards the viscosity solution of (1) as $\Delta\to 0$ under the CFL condition*

$$\lambda\frac{\|\eta\|_\infty}{|\tilde\beta|}\le\theta\le\frac{1}{2},$$

and the additional stability assumption: $\forall(j,n)\in\mathbb{Z}\times\mathbb{N}$,

$$\min_{x\in[x_{j-1},x_{j+1}]}\eta(t^{n+1},x)\ge\max_{x\in[x_{j-1},x_{j+1}]}\eta(t^n,x)\times\left(1+\frac{\Delta t}{\tilde\beta}\max_{x\in[x_{j-1},x_{j+1}]}|\partial_x\eta(t^n,.)|\right),\tag{32}$$

where $\tilde\beta>0$ is the smallest number such that

$$\inf_{j\in\mathbb{Z}}\left[\min_{x\in[x_{j-1},x_{j+1}]}\eta(0,x)-\max\left(\left|\frac{\varphi_j^0-\varphi_{j-1}^0}{\Delta x}\right|,\left|\frac{\varphi_{j+1}^0-\varphi_j^0}{\Delta x}\right|\right)\right]\ge\tilde\beta.\tag{33}$$

Remark 6. The assumptions of Theorem 5 ensure that the CFL condition is meaningful. Notice that (33) is actually a discrete analogue of the inequality (26) in the continuous case.

Proof of Theorem 7. The first step is to establish that, under the restrictions (31) and (32), the inequality (33) holds true for all $n\in\mathbb{N}$. It is therefore convenient to denote by $v^\Delta(t,x)=v_j^n$ for $(t,x)\in T_j^n$ the following "discrete x-derivative" of φ^Δ defined by

$$v_j^n=\frac{\varphi_j^n-\varphi_{j-1}^n}{\Delta x}.\tag{34}$$

We prove by induction on n that the following holds:

$$\inf_{j\in\mathbb{Z}}\left[\min_{x\in[x_{j-1},x_{j+1}]}\eta(t^n,x)-\max\left(|v_j^n|,|v_{j+1}^n|\right)\right]\ge\tilde\beta>0.\tag{35}$$

It is clear that v_j^n is given by the following scheme:

$$v_j^{n+1}=v_j^n-\lambda\Big[\mathsf{H}^{LF}(t^n,x_j,v_j^n,v_{j+1}^n)-\mathsf{H}^{LF}(t^n,x_{j-1},v_{j-1}^n,v_j^n)\Big].\tag{36}$$

Because of the smoothness of $(x,p) \mapsto \mathcal{H}(t,x,p)$ we get by the mean-value theorem that, for some $\bar{x}_j \in [x_{j-1}, x_j]$,

$$v_j^{n+1} = v_j^n - \frac{\lambda}{2}\Big[\Big(\mathcal{H}(t^n, x_j, v_{j+1}^n) - \mathcal{H}(t^n, x_j, v_j^n)\Big) + \Big(\mathcal{H}(t^n, x_{j-1}, v_j^n) - \mathcal{H}(t^n, x_{j-1}, v_{j-1}^n)\Big)\Big] + \frac{\theta}{2}(v_{j+1}^n - 2v_j^n + v_{j-1}^n) + \Delta t \partial_x \mathcal{H}(t^n, \bar{x}_j, v_j^n).$$

We first notice that the afore equality is meaningful, because

$$\partial_x \mathcal{H}(t^n, \bar{x}_j, v_j^n) = -\frac{\eta(t^n, \bar{x}_j)\partial_x \eta(t^n, \bar{x}_j)}{\sqrt{\eta^2(t^n, \bar{x}_j) - (v_j^n)^2}} \tag{37}$$

is well-defined under condition (33).

We introduce the classical incremental coefficients of Harten [18]:

$$\begin{cases} m_{j+\frac{1}{2}}^n = \dfrac{\theta}{\lambda} - \dfrac{\mathcal{H}(t^n, x_j, v_{j+1}^n) - \mathcal{H}(t^n, x_j, v_j^n)}{v_{j+1}^n - v_j^n}, \\ p_{j-\frac{1}{2}}^n = \dfrac{\theta}{\lambda} + \dfrac{\mathcal{H}(t^n, x_{j-1}, v_j^n) - \mathcal{H}(t^n, x_{j-1}, v_{j-1}^n)}{v_j^n - v_{j-1}^n}. \end{cases}$$

The scheme on $(v_j^n)_{(j,n)\in\mathbb{Z}\times\mathbb{N}}$ rewrites after rearrangement:

$$v_j^{n+1} = \Big[1 - \frac{\lambda}{2}(m_{j+\frac{1}{2}}^n + p_{j-\frac{1}{2}}^n)\Big] v_j^n + \frac{\lambda}{2} m_{j+\frac{1}{2}}^n v_{j+1}^n + \frac{\lambda}{2} p_{j-\frac{1}{2}}^n v_{j-1}^n + \Delta t \partial_x \mathcal{H}(t^n, \bar{x}_j, v_j^n).$$

Restriction (31) ensures that the coefficients of the terms v_{j-1}^n, v_j^n and v_{j+1}^n are nonnegative, so that, multiplying the last expression by $\operatorname{sgn}(v_j^{n+1})$, we obtain (see also the proof of Lemma 1 in [17]):

$$|v_j^{n+1}| \le \Big[1 - \frac{\lambda}{2}(m_{j+\frac{1}{2}}^n + p_{j-\frac{1}{2}}^n)\Big] |v_j^n| + \frac{\lambda}{2} m_{j+\frac{1}{2}}^n |v_{j+1}^n| + \frac{\lambda}{2} p_{j-\frac{1}{2}}^n |v_{j-1}^n| + \Delta t |\partial_x \mathcal{H}(t^n, \bar{x}_j, v_j^n)|.$$

Now, let $y \in [x_{j-1}, x_{j+1}]$; we have

$$\begin{aligned} |v_j^{n+1}| - \eta(t^{n+1}, y) \le{} & \Big[1 - \frac{\lambda}{2}(m_{j+\frac{1}{2}}^n + p_{j-\frac{1}{2}}^n)\Big] \Big(|v_j^n| - \eta(t^n, x_j)\Big) \\ & + \frac{\lambda}{2} m_{j+\frac{1}{2}}^n \Big(|v_{j+1}^n| - \eta(t^n, x_j)\Big) \\ & + \frac{\lambda}{2} p_{j-\frac{1}{2}}^n \Big(|v_{j-1}^n| - \eta(t^n, x_j)\Big) \\ & + \Delta t |\partial_x \mathcal{H}(t^n, \bar{x}_j, v_j^n)| + \Big(\eta(t^n, x_j) - \eta(t^{n+1}, y)\Big). \end{aligned}$$

Here we have used the positivity of the incremental coefficients to rewrite $\eta(t^n, x_j)$ as some convex combination. Now we can apply (35) and (37) together with the inequality $0 \le |a| - |b| \le \sqrt{a^2 - b^2}$ in order to obtain

$$|v_j^{n+1}| - \eta(t^{n+1}, y) \le -\tilde{\beta} + \Delta t\, \eta(t^n, \bar{x}_j) \frac{|\partial_x \eta(t^n, \bar{x}_j)|}{\tilde{\beta}} + \left(\eta(t^n, x_j) - \eta(t^{n+1}, y)\right).$$

Under condition (32), the sum of the last three terms in this inequality

is clearly nonpositive, so that we have, for all $y \in [x_{j-1}, x_{j+1}]$, $|v_j^{n+1}| - \eta(t^{n+1}, y) \le -\tilde{\beta}$. The first step of this proof is completed by considering the scheme for v_{j+1}^{n+1}.

The second and last step of the proof merely consists in observing that, on the domain $p < \|\eta\|_\infty$, which is stable by both the equation and its discrete version, the Hamiltonian is C^2 in all the variables. Therefore, all the previous requirements are fulfilled with, e.g., $C = \|\eta\|_\infty(\|\partial_t \eta\|_\infty + \|\partial_x \eta\|_\infty)/|\tilde{\beta}|$ and $M = (\|\eta\|_\infty/|\tilde{\beta}| + \theta/\lambda)$. The CFL restriction is a straightforward consequence of (31). □

4.2 The discrete semiconcavity of LxF type approximations

We want now to mimic at the numerical level the semiconcavity estimate shown in Lemma 1 for the continuous viscosity solution. This is the main reason why we restricted ourselves to simple schemes such as the Lax-Friedrichs type ones, since, up to our knowledge, this property is still unproven for general monotone schemes even in an homogeneous context (see for instance [8, 42, 25]). For some more results concerning other schemes, we refer to [30]. Concerning the multi-dimensional case, we refer again to Lin and Tadmor [27]: their results hold true under strong convexity assumptions on $\mathcal{H}$, which are not necessarily satisfied in our context.

Lemma 3 *Assume that, in addition to the hypotheses of Lemma 1, the following stronger CFL restriction holds:*

(38)

$$\lambda \left[\sup_{\substack{(t,x)\in[0,T]\times\mathbb{R} \\ |p|\le R}} \left|\partial_p \mathcal{H}(t,x,p)\right| + \Delta x \sup_{\substack{(t,x)\in[0,T]\times\mathbb{R} \\ |p|\le R}} \left|\partial_{xp} \mathcal{H}(t,x,p)\right| \right] \le \theta \le \frac{1}{2}.$$

Then the sequence $(\varphi_j^n)_{(j,n)\in\mathbb{Z}\times\mathbb{N}}$ *generated by the scheme (29), (30) satisfies the discrete semiconcavity estimate*

(39) $$\sup_{(j,n)\in\mathbb{Z}\times\mathbb{N}} \left[\max\left(0, \varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n\right)\right] \le \bar{K} \Delta x^2$$

for a constant $\bar{K} \in \mathbb{R}^+$ depending only on R and φ^0.

Remark 7. The forthcoming proof extends to general C^2 Hamiltonians $(t, x, p) \mapsto H(t, x, p)$ strictly convex in the p variable. The difficulty is once again to handle the explicit dependance of $\mathcal{H}$ in x without assuming a strict convexity in both x and p variables. Under this last stronger (and unrealistic!) assumption, one would recover the classical t^{-1} decay for homogeneous problems (see e.g. [23,27,28]).

Proof of Lemma 3. We are actually going to work with the v_j^n quantities (34). Inequality (39) becomes therefore a *weak discrete OSLC property* in the sense of Brenier and Osher [8] (see also the early proof by Smoller in [38], and [42]). We proceed by induction, dropping the variable t^n in $\mathcal{H}$ for the sake of clarity. Setting $z_j^n = (v_{j+1}^n - v_j^n)/\Delta x$, we obtain from (36):

$$\begin{aligned} z_j^{n+1} = \frac{\theta}{2} z_{j+1}^n + (1-\theta) z_j^n + \frac{\theta}{2} z_{j-1}^n \\ -\frac{\lambda}{2\Delta x}\Big[\Big(\mathcal{H}(x_j, v_{j+1}^n) - \mathcal{H}(x_{j-1}, v_j^n)\Big) \\ +\Big(\mathcal{H}(x_j, v_j^n) - \mathcal{H}(x_{j-1}, v_{j-1}^n)\Big) \\ -\Big(\mathcal{H}(x_{j-1}, v_j^n) - \mathcal{H}(x_{j-2}, v_{j-1}^n)\Big) \\ -\Big(\mathcal{H}(x_{j-1}, v_{j-1}^n) - \mathcal{H}(x_{j-2}, v_{j-2}^n)\Big)\Big]. \end{aligned}$$

We use Taylor expansions up to second derivatives to treat each difference inside the parentheses. The trick is to do that in such a way that the $\partial_x \mathcal{H}$ terms can be recombined (the variables ξ_j^n, $\bar{x}_{j-\frac{1}{2}}$, $\tilde{x}_{j-\frac{1}{2}}$ in the following are intermediate points introduced by second order Taylor expansions):

$$\begin{aligned} \mathcal{H}(x_j, v_{j+1}^n) - \mathcal{H}(x_{j-1}, v_j^n) = \Delta x\, \partial_x \mathcal{H}(x_{j-1}, v_{j+1}^n) \\ + \frac{\Delta x^2}{2} \partial_{xx} \mathcal{H}(\bar{x}_{j-\frac{1}{2}}, v_{j+1}^n) \\ + \Delta x\, z_{j+1}^n \partial_p \mathcal{H}(x_{j-1}, v_j^n) \\ + \frac{\Delta x^2}{2} (z_{j+1}^n)^2 \partial_{pp} \mathcal{H}(x_{j-1}, \xi_{j+1}^n), \end{aligned}$$

$$\begin{aligned} \mathcal{H}(x_j, v_j^n) - \mathcal{H}(x_{j-1}, v_{j-1}^n) = \Delta x\, \partial_x \mathcal{H}(x_{j-1}, v_j^n) \\ + \frac{\Delta x^2}{2} \partial_{xx} \mathcal{H}(\tilde{x}_{j-\frac{1}{2}}, v_j^n) \\ + \Delta x\, z_j^n \partial_p \mathcal{H}(x_{j-1}, v_{j-1}^n) \\ + \frac{\Delta x^2}{2} (z_j^n)^2 \partial_{pp} \mathcal{H}(x_{j-1}, \xi_j^n), \end{aligned}$$

$$\begin{aligned}\mathcal{H}(x_{j-1},v_j^n)-\mathcal{H}(x_{j-2},v_{j-1}^n)&=\Delta x\,\partial_x\mathcal{H}(x_{j-1},v_{j-1}^n)\\&+\frac{\Delta x^2}{2}\partial_{xx}\mathcal{H}(\bar{x}_{j-\frac{3}{2}},v_{j-1}^n)\\&+\Delta x\,z_j^n\partial_p\mathcal{H}(x_{j-1},v_j^n)\\&+\frac{\Delta x^2}{2}(z_j^n)^2\partial_{pp}\mathcal{H}(x_{j-1},\tilde{\xi}_j^n),\end{aligned}$$

$$\begin{aligned}\mathcal{H}(x_{j-1},v_{j-1}^n)-\mathcal{H}(x_{j-2},v_{j-2}^n)&=\Delta x\,\partial_x\mathcal{H}(x_{j-1},v_{j-2}^n)\\&+\frac{\Delta x^2}{2}\partial_{xx}\mathcal{H}(\tilde{x}_{j-\frac{3}{2}},v_{j-2}^n)\\&+\Delta x\,z_{j-\frac{1}{2}}^n\partial_p\mathcal{H}(x_{j-1},v_{j-1}^n)\\&+\frac{\Delta x^2}{2}\,(z_{j-\frac{1}{2}}^n)^2\partial_{pp}\mathcal{H}(x_{j-1},\tilde{\xi}_{j-1}^n).\end{aligned}$$

Now to get rid of the terms involving $\partial_x\mathcal{H}$, we use the mean-value theorem with a $\zeta_{j+\frac{1}{2}}\in]x_j,x_{j+1}[$:

$$\begin{aligned}&\partial_x\mathcal{H}(x_{j-1},v_{j+1}^n)-\partial_x\mathcal{H}(x_{j-1},v_{j-1}^n)\\&\quad=\Delta x\,z_{j+1}^n\partial_{xp}\mathcal{H}(x_{j-1},\zeta_{j+\frac{1}{2}}^n)+\Delta x\,z_j^n\partial_{xp}\mathcal{H}(x_{j-1},\zeta_{j-\frac{1}{2}}^n).\end{aligned}$$

Using a similar expansion for the difference between v_j^n and v_{j-2}^n leads to a new expression for z_j^{n+1}:

$$\begin{aligned}z_j^{n+1}=&\frac{1}{2}z_{j+1}^n\Big(\theta-\lambda\Big[\partial_p\mathcal{H}(x_{j-1},v_j^n)+\Delta x\,\partial_{xp}\mathcal{H}(x_{j-1},\zeta_{j+\frac{1}{2}}^n)\Big]\Big)\\&+z_j^n\Big(1-\theta-\frac{\lambda}{2}\Big[\partial_p\mathcal{H}(x_{j-1},v_{j-1}^n)-\partial_p\mathcal{H}(x_{j-1},v_j^n)\\&+\Delta x\,\partial_{xp}\mathcal{H}(x_{j-1},\zeta_{j-\frac{1}{2}}^n)+\Delta x\,\partial_{xp}\mathcal{H}(x_{j-1},\bar{\zeta}_{j-\frac{1}{2}}^n)\Big]\Big)\\&+\frac{1}{2}z_{j-1}^n\Big(\theta+\lambda\Big[\partial_p\mathcal{H}(x_{j-1},v_{j-1}^n)-\Delta x\,\partial_{xp}\mathcal{H}(x_{j-1},\bar{\zeta}_{j-\frac{3}{2}}^n)\Big]\Big)\\&-\frac{\Delta t}{4}\Big[\partial_{pp}\mathcal{H}(x_{j-1},\xi_{j+1}^n)(z_{j+1}^n)^2+\Big(\partial_{pp}\mathcal{H}(x_{j-1},\xi_j^n)\\&+\partial_{pp}\mathcal{H}(x_{j-1},\tilde{\xi}_j^n)\Big)(z_j^n)^2+\partial_{pp}\mathcal{H}(x_{j-1},\tilde{\xi}_{j-1}^n)(z_{j-1}^n)^2\Big]\\&-\frac{\Delta t}{4}\Big[\partial_{xx}\mathcal{H}(\bar{x}_{j-\frac{1}{2}},v_{j+1}^n)+\partial_{xx}\mathcal{H}(\tilde{x}_{j-\frac{1}{2}},v_j^n)\\&+\partial_{xx}\mathcal{H}(\bar{x}_{j-\frac{3}{2}},v_{j-1}^n)+\partial_{xx}\mathcal{H}(\tilde{x}_{j-\frac{3}{2}},v_{j-2}^n)\Big].\end{aligned}$$

We introduce now the quantity we are interested in, namely $y_j^n=\max(0,z_j^n)$. We notice that $y_j^n\geq z_j^n$ and $(y_j^n)^2\leq(z_j^n)^2$. The coefficients of the square terms are negative because of (22), and, under the stronger CFL condition (38), the coefficients of the linear terms are nonnegative, so that we can replace z_{j-1}^n , z_j^n z_{j+1}^n respectively by y_{j-1}^n , y_j^n y_{j+1}^n and obtain an upper bound for z_j^{n+1}. Next, we replace y_j^n by

$$\tilde{y}_j^n = \max(y_{j-1}^n, y_j^n, y_{j+1}^n),$$

and the same kind of argument gives once again an upper bound. In doing so, the $\partial_p \mathcal{H}$ terms cancel, and we are left only with second derivatives of $\mathcal{H}$, for which we have bounds (see the definitions (22)-(25) of the coefficients $\zeta_0, \zeta_1, \zeta_2$). We end up with

$$z_j^{n+1} \leq \tilde{y}_j^n - \zeta_0 \Delta t (\tilde{y}_j^n)^2 - 2\zeta_1 \Delta t \tilde{y}_j^n - \zeta_2 \Delta t.$$

In order to use monotonicity, we need to perform a slight adjustment to take into account the *a priori* bounds on y_j^n. Indeed, we have

$$z_j^n \leq |z_j^n| \leq \frac{2 \sup_j |v_j^n|}{\Delta x} \leq \frac{2M}{\Delta x} \leq \frac{2M}{A \Delta t},$$

where

$$A = \sup_{(t,x) \in [0,T] \times \mathbb{R}; |p| \leq M} |\partial_p \mathcal{H}(t,x,p)| + \Delta x \sup_{(t,x) \in [0,T] \times \mathbb{R}; |p| \leq M} |\partial_{xp} \mathcal{H}(t,x,p)|,$$

and the last inequality follows from the CFL condition. The same inequality holds for y_j^n. Now we introduce the adjusted coefficient $\tilde{\zeta}_0 = \min\left(\zeta_0, \frac{A}{2M}\right)$, so that $0 < \tilde{\zeta}_0 \leq \zeta_0$, and we define $F(y) = y - \tilde{\zeta}_0 \Delta t y^2 - 2\zeta_1 \Delta t y - \zeta_2 \Delta t$. We still have $z_j^{n+1} \leq F(\tilde{y}_j^n)$. The function F is nondecreasing for $y \leq \frac{1 - 2\zeta_1 \Delta t}{2\tilde{\zeta}_0 \Delta t}$, which contains the range of y_j^n. Therefore, since $\tilde{y}_j^n \geq 0$, we have $F(\tilde{y}_j^n) \geq F(0) = -\zeta_2 \Delta t \geq 0$ (since $\zeta_2 \leq 0$), and this implies $y_j^{n+1} \leq F(\tilde{y}_j^n)$. Setting $M^n = \sup_{j \in \mathbb{Z}} \tilde{y}_j^n$, we have by monotonicity $F(\tilde{y}_j^n) \leq F(M^n)$, and, taking the supremum over $j \in \mathbb{Z}$, $M^{n+1} \leq F(M^n)$.

We conclude exactly in the same way as in the continuous case (Lemma 1), by just noticing that F has two real roots $X_- \leq 0 \leq X_+$, and the result easily follows if we set $\bar{K} = \max(M^0, X_+)$. □

Remark 8. From the discrete semiconcavity estimate, we can obtain, in the same spirit as in the continuous case, a convergence estimate for the numerical solution. Indeed, the decay of the L^1 norm of the difference is of order Δx (see [27]). This has been numerically evidenced in [17] (see Fig. 4.1) on a Burgers equation, with a modified Lax-Friedrichs type scheme as used in Sect. 5 ($\theta = 1/2$). This leads to the same rate of convergence for the Schrödinger equation with $V = 0$.

The extension of such a proof towards general *monotone* Hamiltonians does not seem to be straightforward. In fact, one of its crucial ingredients is the use of a constant artificial viscosity coefficient θ, that allows to work extensively with $\mathcal{H}$ for which we have all the desired properties. The case of similar schemes with variable values $\theta^n_{j+\frac{1}{2}}$ remains misty, as Godunov type schemes which lead moreover to more intricate formulæ. The result is likely to be true; however, we have no rigorous proof to state at this time. Finally, upwind-type schemes (see e.g. [36]) cannot be treated within the same approach because of the lack of smoothness of their numerical Hamiltonians involving some discontinuous min/max functions.

To summarize, we just say now that, under the reinforced CFL condition (38) (which obviously implies the standard one (31)), for both the Schrödinger equation and the Helmholtz equation, we have

– the numerical solutions computed by the Lax-Friedrichs scheme converge to the viscosity solution;
– they satisfy moreover a discrete semiconcavity estimate.

Lemma 3 directly applies for the Hamiltonian deduced from the Schrödinger equation.

4.3 Upwind schemes for the linear conservation equation

To investigate the behaviour of the numerical schemes for the linear conservation equation, we will mainly rely on a previous work [16] in which very general schemes have been studied. The general form of a linear conservative $(2K+1)$-points scheme can be written

(40)
$$\begin{cases} \mu_j^{n+1} = \mu_j^n - \dfrac{\Delta t}{\Delta x}\left(< \mathbf{A}^n_{j+\frac{1}{2}}, \boldsymbol{\mu}^n_{j+\frac{1}{2}} >_{\mathbb{R}^{2K}} - < \mathbf{A}^n_{j-\frac{1}{2}}, \boldsymbol{\mu}^n_{j-\frac{1}{2}} >_{\mathbb{R}^{2K}} \right) \\ \boldsymbol{\mu}^n_{j+\frac{1}{2}} = \left(\mu^n_{j-K+1}, \dots, \mu^n_{j+K} \right) \in \mathbb{R}^{2K} \\ \mathbf{A}^n_{j+\frac{1}{2}} = \left(a^n_{j+\frac{1}{2},-K+1}, \dots, a^n_{j+\frac{1}{2},K} \right) \in \mathbb{R}^{2K} \end{cases}$$

In this formula, $< \cdot, \cdot >_{\mathbb{R}^{2K}}$ stands for the standard scalar product in $\mathbb{R}^{2K}$. The scheme is completely determined as soon as the coefficients $\mathbf{A}^n_{j+\frac{1}{2}}$ are specified. Our convergence results, [16], are valid for any K; however, for practical computations, we used three- points schemes, that is $K = 1$. In [16], several examples of $\mathbf{A}^n_{j+\frac{1}{2}}$ corresponding to classical schemes have been investigated. After comparisons between several of them, it turned out that the best performances were obtained with upwind discretizations. Therefore we shall limit ourselves to such schemes in the following.

The sequence μ_j^n naturally gives rise to a family of piecewise constant functions μ^Δ by setting

$$\mu^\Delta(t,x) = \mu_j^n \qquad \text{for} \quad (t,x) \in T_j^n.$$

When $\Delta \to 0$, this sequence eventually converges to a measure in the space variable. Therefore, we assume that $\mu^\Delta(0,.) \rightharpoonup \mu^0$ as $\Delta x \to 0$ in the weak topology of measures. This is achieved for instance by defining μ_j^0 as the local average of μ^0 on $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}[$.

We recall that the convergence of the numerical solution generated by such a scheme relies on the following properties (see [16] for details). First, one has to ensure that, according to the notations of (40), the set of coefficients

$$\begin{cases} B_{j,-1}^n = C_{j,-1}^n = \lambda a_{j+\frac{1}{2},0}^n \\ B_{j,0}^n = 1 + \lambda\Big(a_{j-\frac{1}{2},1}^n - a_{j+\frac{1}{2},0}^n\Big) \\ C_{j,0}^n = 1 + \lambda\Big(a_{j+\frac{1}{2},1}^n - a_{j+\frac{1}{2},0}^n\Big) \\ B_{j,1}^n = C_{j,1}^n = -\lambda a_{j-\frac{1}{2},1}^n \end{cases} \tag{41}$$

are nonnegative. Next, the so-called **weak consistency** of the scheme has to be established. For this, we need the piecewise constant functions: for $(t,x) \in T_j^n$,

$$a^\Delta(t,x) = a_{j+\frac{1}{2},0}^n + a_{j+\frac{1}{2},1}^n,$$
$$b^\Delta(t,x) = \frac{1}{\Delta x}\left[(a_{j-\frac{1}{2},0}^n - a_{j-\frac{3}{2},0}^n) + (a_{j+\frac{1}{2},1}^n - a_{j-\frac{1}{2},1}^n)\right].$$

The scheme is said to be weakly consistent if $a^\Delta \rightharpoonup a$ in $L^\infty(]0,T[\times\mathbb{R})$ weak $\star$ as $\Delta \to 0$, and if $b^\Delta \leq \alpha^\Delta$ for some $\alpha^\Delta \in L^1(]0,T[)$.

The key point for all examples is of course the choice of the discretization of $\partial_x\varphi$. According to Lemma 3, it is clearly convenient to consider *convex combinations* of the adjacent quantities $(\varphi_{j+1}^n - \varphi_j^n)/\Delta x$. Therefore, in order to take advantage of the discrete semiconcavity property (39), we define:

$$D\varphi_{j+\frac{1}{2}}^n = \sum_{i=-I_0}^{I_0} \ell_i \frac{\varphi_{j+i+1}^n - \varphi_{j+i}^n}{\Delta x}, \qquad \text{with } \ell_i \geq 0, \sum_{i=-I_0}^{I_0} \ell_i = 1. \tag{42}$$

This general definition permits to recover for instance the particular value of $D\varphi_{j+\frac{1}{2}}^n$ proposed in [14]: $I_0 = 1$, $\ell_{\pm 1} = 1/4$, $\ell_0 = 1/2$. But it does not allow to recover the rough "Engquist-Osher type" upwind scheme tested in [16]. This is not a genuine drawback since this discretization would generate spurious spikes in the neighborood of the local minimum points of the phase φ (see Fig. 5 in [15]).

In the case of the Schrödinger equation, we propose the upwind scheme simply defined by:

$$\mathbf{A}^n_{j+\frac{1}{2}} = \Big(\max\big(0, D\varphi^n_{j+\frac{1}{2}}\big), \min\big(0, D\varphi^n_{j+\frac{1}{2}}\big)\Big). \tag{43}$$

Theorem 8 *(numerical convergence for the Schrödinger equation) Under the assumptions of Theorems 4 and 6, the sequence* $(\varphi^\Delta, \mu^\Delta)$ *converges as* $\Delta \to 0$ *towards the unique couple* (φ, μ) *of viscosity/duality solutions to (21).*

Proof. We have shown that the sequence φ^Δ converges to the viscosity solution. This implies that a^Δ converges strongly in $L^1_{loc}(]0,T[\times\mathbb{R})$ to $a = \partial_x\varphi$ (see Theorems 1.1 and 2.2 in [9]). Next, the strong CFL condition (38) is trivially satisfied by the Hamiltonian $p^2/2$, so a discrete semiconcavity estimate holds. Therefore, the second assertion in the weak consistency definition is saitisfied with $\alpha^\Delta = 4\bar{K}$. Finally, the nonnegativity of the coefficients B^n_j, C^n_j is enforced by the CFL conditions. □

Now, concerning the Helmholtz equation, we propose

$$\mathbf{A}^n_{j+\frac{1}{2}} = \left(\frac{\max\Big(0, D\varphi^n_{j+\frac{1}{2}}\Big)}{(\varphi^{n+1}_j - \varphi^n_j)/\Delta t}, \frac{\min\Big(0, D\varphi^n_{j+\frac{1}{2}}\Big)}{(\varphi^{n+1}_{j+1} - \varphi^n_{j+1})/\Delta t} \right), \tag{44}$$

together with the preceding choice for $D\varphi^n_{j+\frac{1}{2}}$. This is obviously not the unique possibility.

We have to ensure that the approximation of $\partial_t\varphi$ remains strictly positive. This was easy at the level of the continuous equation. Here we have to take care of the numerical viscosity. This is the purpose of the following lemma.

Lemma 4 *Under the assumptions of Theorem 5, the hypotheses (32), (33), the stronger CFL condition (38), the coefficients* $\mathbf{A}^n_{j+\frac{1}{2}}$ *are well-defined and bounded for all* $n \in \mathbb{N}, j \in \mathbb{Z}$*, provided the following restriction holds: there exists* $\kappa > \eta_0 - \tilde{\beta} \geq 0$ *such that*

$$\forall j \in \mathbb{Z}, \quad \mathsf{H}^{LF}\left(0, x_j, \frac{\varphi^0_j - \varphi^0_{j-1}}{\Delta x}, \frac{\varphi^0_{j+1} - \varphi^0_j}{\Delta x}\right) \leq -\kappa. \tag{45}$$

Remark 9. Conditions (33) and (45) are somehow two discrete versions of (26). Condition (45) is a slight refinement taking into account the numerical viscosity involved in the numerical Hamiltonian H^{LF}.

The constants κ and $\tilde{\beta}$ depend on the initial data and the refraction index. For instance, provided the initial datum for the phase is $W^{2,\infty}$, then (45) is a consequence of (26), with $\kappa = \tilde{\beta} + \|\partial_{xx}\varphi^0\|_\infty$. If the initial phase is constant, which is the case in the computations presented in Sect. 5, (45) holds with $\kappa = \tilde{\beta} = \inf_{x\in\mathbb{R}} \eta(0,x) = \eta_0$.

Proof of Lemma 4. We introduce two notations. First we set

$$\mathcal{H}_k^n = \Big(\mathcal{H}(t^n, x_k, v_k^n) + \mathcal{H}(t^n, x_{k+1}, v_{k+1}^n)\Big)/2,$$

so that, from the assumption $\eta \geq \eta_0$ and (33), (35) we have for all k, n, $-\eta_0 \leq \mathcal{H}_k^n \leq \tilde{\beta}$. Next, we shall use

$$\mathbf{H}_j^n = -\mathsf{H}^{LF}(t^n, x_j, v_j^n, v_{j+1}^n) = (\varphi_j^{n+1} - \varphi_j^n)/\Delta t.$$

We have to prove that $\mathbf{H}_j^n \geq \alpha > 0$ for all $j, n \in \mathbb{Z}\times\mathbb{N}$. We proceed by induction on n, and first notice that, if (45) holds, then we have:

$$\mathbf{H}_j^0 + \inf_{k\in\mathbb{Z}} \mathcal{H}_k^0 \geq \kappa - \eta_0. \tag{46}$$

We claim that this inequality propagates for all $n \in \mathbb{N}$. Indeed, we have for any $j, k \in \mathbb{Z}^2$

$$\begin{aligned}\mathbf{H}_j^{n+1} + \mathcal{H}_k^{n+1} &= \mathbf{H}_j^n + \mathcal{H}_k^n + \frac{\theta}{2}\mathbf{H}_{j+1}^n - \theta\mathbf{H}_j^n + \frac{\theta}{2}\mathbf{H}_{j-1}^n \\ &= \frac{\theta}{2}\Big(\mathbf{H}_{j+1}^n + \mathcal{H}_k^n\Big) + (1-\theta)\Big(\mathbf{H}_j^n + \mathcal{H}_k^n\Big) \\ &\quad + \frac{\theta}{2}\Big(\mathbf{H}_{j-1}^n + \mathcal{H}_k^n\Big).\end{aligned}$$

Consequently, if the inequality (46) holds true for any n, then we get the expected result at the next step $n+1$. Therefore, we have that, for all k, $\mathbf{H}_j^n \geq \kappa - \eta_0 - \mathcal{H}_k^n \geq \kappa - \eta_0 + \tilde{\beta} \equiv \alpha > 0$. □

Now we state a convergence theorem for the Helmholtz equation.

Theorem 9 *(numerical convergence for the Helmholtz equation)*
Under the assumptions of Theorem 5, the sequence of numerical approximations $(\varphi^\Delta, \mu^\Delta)$ generated by the class of schemes (29), (30), (40), (42), (44) converges as $\Delta \to 0$ to the unique couple of viscosity/duality solutions of the system (21), provided η and $\varphi^\Delta(0,.)$ satisfy the requirements (32), (33), (45), and the following CFL conditions hold:

$$\lambda\frac{\|\eta\|_\infty}{|\tilde{\beta}|}\left(1 + \Delta x\frac{\|\eta\|_\infty \cdot Lip(\eta)}{\tilde{\beta}^2}\right) \leq \theta \leq \frac{1}{2},$$

$$\lambda\frac{\|\eta\|_\infty}{|\kappa|} \leq \frac{1}{2}. \tag{47}$$

Proof. The proof is a direct consequence of Theorem 7 and Lemmas 3, 4. First, it is straightforward to see that the CFL condition (47) ensures both the semiconcavity requirement (38) and the nonnegativity of the coefficients B_j^n, C_j^n (41). Next, as for the case of the Schrödinger equation, the convergence of φ^Δ ensures the weak convergence of a^Δ, and, finally, using the inequality $\frac{a}{b} - \frac{c}{d} \leq \frac{1}{b}(a-c) + |c|(\frac{1}{|b|} + \frac{1}{|d|})$, we find a constant upper bound for b^Δ, namely $C = \frac{4}{|\kappa|}(\bar{K} + \|\eta\|_\infty)$. □

5 Numerical results

In this section, we display standard test-cases for this kind of problems. They all have been already studied for instance in [13–15, 20, 37]. We refer the reader to these papers for any comparison with our results. All our computations have been carried out on the same domain, namely the square $x \in [-1, 1]$, $t \in [0, 2]$. The parameters are $\Delta x = 0.04$ and $\Delta t = 0.02$. We chosed the upper bound $\theta = \frac{1}{2}$ in (29) corresponding to Tadmor's modification [43] of the classical Lax-Friedrichs scheme. Finally, we took $I_0 = 0$, $\ell_0 = 1$ in (42).

5.1 The Schrödinger equation

We give two examples selected from [20]. One of them leads to smooth solutions, while the other one is focusing, and generates three phases after a finite time. We compute in this last case a Dirac mass.

We consider the case of the free Schrödinger equation, that is $V(x) \equiv 0$. The data are the following: the amplitude is the same in both cases, namely $A(0, x) = \exp(-x^2)$. The initial phases are chosen $\varphi(0, x) = \pm\ln(\cosh(x))$, the plus sign corresponds to the expansive case. The results are displayed in Figs. 1 and 2.

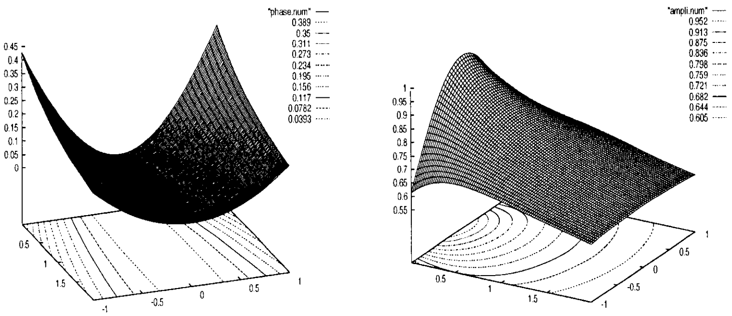

Fig. 1. Numerical phases and amplitudes: Schrödinger equation (expansive case)

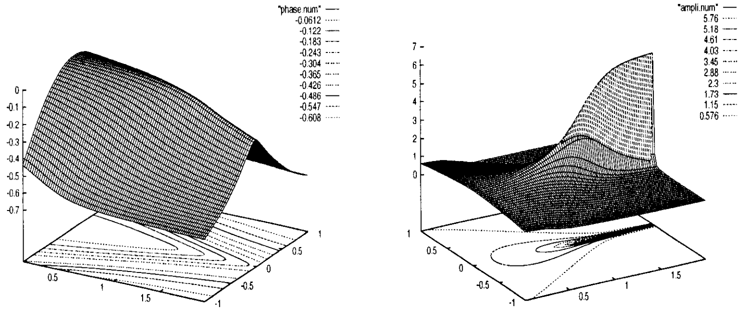

Fig. 2. Numerical phases and amplitudes: Schrödinger equation (compressive case)

5.2 The Helmholtz equation

For all the computations in this case, the initial data are

$$\forall x \in \mathbb{R}, \quad \varphi(0,x) \equiv 0, \quad A(0,x) \equiv 1.$$

The various analytical expressions for η are taken from [15, 37].

A concave lens. We simulate a concave lens by choosing the refraction index η the following way:

$$\eta(t,x) = \begin{cases} \dfrac{4}{3 - \cos\left(\pi(t-1)/E\right)} & \text{if } D < 1, \\ 1 \text{ in the other cases,} & \end{cases} \tag{48}$$

$$\text{where} \qquad D = \left(\frac{t-1}{0.3}\right)^2 - \left(\frac{x}{0.8}\right)^2, \quad E = 0.3\sqrt{1 + \left(\frac{x}{0.8}\right)^2}.$$

Since the viscosity solution turns out to be differentiable in the whole computational domain, we end up with a global smooth solution which is actually a correct approximation of the infinite frequency expansion of the Helmholtz solution [45] (see Fig. 3). The boundary conditions for the phase need a specific treatment: we followed the method proposed in [14].

A smooth wedge. We simulate a smooth wedge by selecting the following value for the refraction index η:

$$\eta(t,x) = 1.5 + \frac{1}{\pi}\arctan\left(10\sqrt{2}(t - 0.2 - |x|)\right) \tag{49}$$

In this case, the growth restriction on η (32) is fulfilled for Δt small enough. We observe on Fig. 4 a shock on the phase φ after a short time $t_0 = 0.2$ and therefore a blow-up on the amplitudes because of the highly compressive nature of $\partial_x \varphi$. In this case, the exact solution of (13) develops strong caustics and two phases are necessary to describe it (see [37] p.79 for a ray-traced solution).

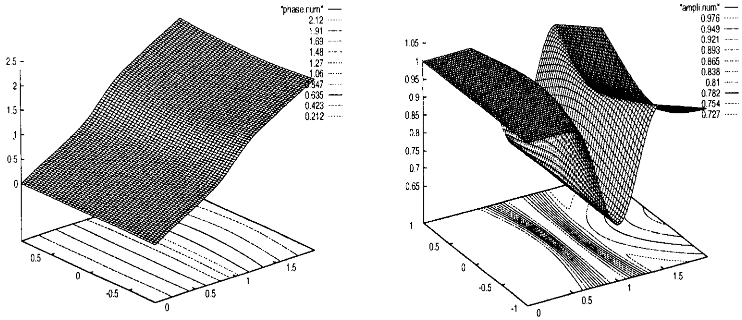

Fig. 3. Numerical values for the phase and the amplitude: the concave lens (48)

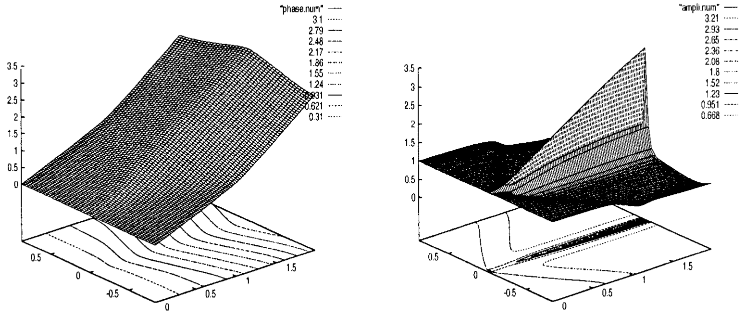

Fig. 4. Numerical values for the phase and the amplitude: smooth wedge (49)

A convex lens. We compute a convex lens with the following values for the refraction index η:

(50)

$$\eta(t,x) = \begin{cases} \dfrac{4}{3-\cos(\pi D)} \text{ if } D < 1 \\ 1 \text{ in the other cases} \end{cases} \quad \text{with } D = \left(\frac{t-1}{0.3}\right)^2 + \left(\frac{x}{0.8}\right)^2 .$$

In this case, we observe on Fig. 5 the classical blow-up for the amplitude of the ansatz on the shock curve of the phase. The exact infinite frequency asymptotics for (13) develop up to five phases around the focal point $(x = 0, t = 1.5)$ and settles with three phases behind this region (see [37] and also [13, 14]).

6 Conclusion

We presented in this paper several convergence results for a nonhomogeneous system one gets out of the geometric optics expansion for several significant examples. The problem has been studied from both theoretical and numerical viewpoints in the context of viscosity and duality solutions. It

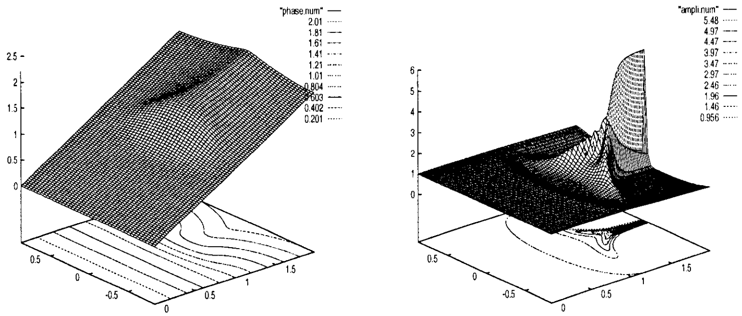

Fig. 5. Numerical values for the phase and the amplitude: the convex lens (50)

turns out that it is possible to give existence and uniqueness results for very general initial data in this class of weak solutions and to establish compactness for sequences of approximations generated by rather natural numerical schemes. Some computational runs demonstrate that this approach is realizable and efficient in several practical situations.

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