NONCLASSICAL RIEMANN SOLVERS WITH NUCLEATION

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Abstract. We introduce a new nonclassical Riemann solver for scalar conservation laws with concave-convex flux-function. This solver is based on both a kinetic relation, which determines the propagation speed of (undercompressive) nonclassical shock waves, and a nucleation criterion, which makes a choice between a classical Riemann solution and a nonclassical one. We establish the existence of (nonclassical entropy) solutions of the Cauchy problem and discuss several examples of wave interactions. We also show the existence of a class of solutions, called splitting-merging solutions, which are made of two large shocks and small BV (bounded variation) perturbations. The nucleation solvers, as we call them, are applied to (and actually motivated by) the theory of thin film flows; they help explain numerical results observed for such flows.

1. Introduction

We introduce the notion of nucleation condition for solutions of the Riemann problem for scalar conservation laws in one space variable,

$$\partial_t u + \partial_x f(u) = 0, \tag{1.1}$$

in which the (smooth) flux-function $f : \boldsymbol{R} \to \boldsymbol{R}$ is nonconvex. The nucleation condition introduced here leads to new behavior of solutions of the Cauchy problem, consisting of equation (1.1) with initial conditions

$$u(x,0) = u_0(x). \tag{1.2}$$

Most notably, (1.1), (1.2) can have multiple attractors, i.e., solutions with different behavior as $t \to +\infty$, corresponding to different data $u_0 : \boldsymbol{R} \to \boldsymbol{R}$, but having the same limits $u_0(\pm\infty)$. The setting we propose covers recent studies of thin film equations [5,6] in which a scalar conservation law with nonconvex flux is regularized by fourth-order diffusion. Indeed, this application motivated the introduction of the nucleation condition.

For scalar conservation laws, *undercompressive shocks* (a term introduced first for non-strictly hyperbolic systems [25]) are propagating discontinuities with characteristics passing

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2000 *Mathematics Subject Classification*. Primary: 35L65, 74XX. Secondary: 76N10, 76L05.

Key words and phrases: hyperbolic, conservation law, shock wave, Riemann solver, undercompressive, nonclassical, nucleation criterion.

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through them. These are to be contrasted with *compressive shocks,* satisfying the Lax entropy inequalities, which have characteristics impinging from both sides. In typical situations, undercompressive shocks have to satisfy the additional condition that they can be associated with traveling wave solutions of a regularized version of (1.1). Consequently, the family of undercompressive shocks for a specific equation (1.1) depends on the details of the regularization.

This additional traveling wave condition can be abstracted, and thus disassociated from the regularization, by embodying it in a so-called *kinetic relation*, an additional condition originally motivated by mechanical considerations for systems of mixed type modeling phase transitions [1,2,16,26,27]. As in [17], we will refer to undercompressive shocks defined through a kinetic relation as *nonclassical shocks.*

For scalar equations, a unique solution of the Riemann problem is obtained by imposing a single entropy inequality and a kinetic relation and by taking the nonclassical solution (i.e., involving nonclassical shocks) whenever it is available; otherwise taking the classical solution (which is always available). Many results are known concerning nonclassical solutions of the Cauchy problem, including existence and uniqueness issues, and generalizations to systems, as described in the book of the first author [17]. Moreover, for conservation laws regularized with second-order diffusion and dispersion, such as the modified KdV-Burgers equation and generalizations [4,11,13,15,17], this appears to be the correct framework. Kinetic relations have also been studied numerically [7,8,12,18]. In particular, using the Glimm's scheme, Chalons and LeFloch [8] studied the time-asymptotics of nonclassical solutions.

For systems of mixed type modeling phase transitions, it is recognized that, on physical grounds, the classical solution should sometimes be selected, even when the nonclassical solution is available. This led Abeyeratne and Knowles [2] to introduce the notion of *nucleation condition,* a rule that selects a unique solution of the Riemann problem, again based on physically reasonable modeling. The issue of nucleation is also considered in [21].

Recent studies of thin film equations [5,6], in which surface tension generates a fourth-order diffusion regularization of a scalar conservation law, have highlighted new behavior that we seek to explain with a nucleation condition for scalar equations. Our purpose in this paper is to introduce the nucleation condition for scalar conservation laws, and to explore some consequences. We are particularly interested in time-asymptotics of nonclassical solutions.

In Section 2, we recall basic notions of entropy dissipation [17], and in Section 3 we introduce a new Riemann solver that incorporates both a kinetic relation and a nucleation condition. The nucleation condition provides a selection mechanism to determine if the evolution is classical or nonclassical. The difference from earlier studies of nonclassical shocks for scalar equations is that previously, there was a continuous transition from classical to nonclassical shocks; in fact, the solution of the Riemann problem was continuous in L^1 with respect to the data [17]. Here, with the new nucleation condition, we lose this continuous dependence, an important departure from standard hyperbolic theory. Nonetheless, we are still able to prove existence of solutions of the Cauchy problem, in Section 4, by the technique of wave front tracking. Indeed, the argument is almost entirely that of the earlier theory [3,17], except that here, the classical solution is sometimes selected when there is an alternative nonclassical solution available, so that solutions involve nonclassical waves less often.

In Section 5, we give three examples that explore consequences of the new Riemann solver. One of our explicit examples leads us, in Section 6, to explore a class of solutions exhibiting repeated wave splitting and merging: an initially classical shock may be split into a nonclassical shock and another classical shock; the two waves can also reunite at a later time. For the convergence analysis we derive uniform bounds on a modified total variation of the wave front tracking solutions. This is achieved by extending a notion in [3,17] and modifying the strength of the nonclassical wave so that the "generalized" total variation is decreasing or continuous at each merging and splitting. We can show that when the nucleation condition is imposed, the total variation decreases by a finite amount at each merging/splitting. Therefore, only finitely many mergings/splittings can take place, which allows us to conclude that asymptotically in time, the solution converges to a single classical shock or else a nonclassical shock and a classical shock.

The connection with the structures observed numerically for thin films is explained in Section 6. We conclude in Section 7 with some discussion of the results and their wider implications.

2. Preliminaries

Consider the scalar conservation law

$$\partial_t u + \partial_x f(u) = 0, \quad u = u(x,t) \in \boldsymbol{R},\ x \in \boldsymbol{R},\ t > 0, \tag{2.1}$$

where $f : \boldsymbol{R} \mapsto \boldsymbol{R}$ is a given smooth flux function. We consider the concave-convex case, in which f satisfies the additional conditions

$$\begin{aligned} &u\, f''(u) > 0 \quad \text{for } u \neq 0, \\ &f'''(0) \neq 0, \qquad \lim_{u \to \pm\infty} f'(u) = +\infty. \end{aligned} \tag{2.2}$$

A **shock wave from** u_- **to** u_+ is defined (in this paper) to be a weak solution $u = u(x,t)$ that is piecewise constant near a discontinuity $x = st + c$, where the shock speed $s = \overline{a}(u_-, u_+)$ is given by the Rankine-Hugoniot condition

$$\overline{a}(u_-, u_+) := \frac{f(u_-) - f(u_+)}{u_- - u_+},$$

c is a real parameter, and $u_\pm := u(st + c\pm, t)$. A shock wave from u_- to u_+ is a **classical shock** if it satisfies the *Lax shock inequalities*

$$f'(u_+) \le \overline{a}(u_-, u_+) \le f'(u_-).$$

We consider equation (2.1) supplemented by a *single* entropy inequality

$$\partial_t U(u) + \partial_x F(u) \le 0 \tag{2.3}$$

in the weak sense, where U, F is a specific entropy-entropy flux pair: $U : \boldsymbol{R} \to \boldsymbol{R}$ is convex and $F : \boldsymbol{R} \to \boldsymbol{R}$ related to U by compatibility with the conservation law (2.1):

$$F'(u) := f'(u)\, U'(u).$$

The entropy inequality (2.3) gives rise to a restriction on shock waves in addition to the Rankine Hugoniot condition. We define the *entropy dissipation function* $E : \boldsymbol{R} \times \boldsymbol{R} \to \boldsymbol{R}$ by

$$E(u_-, u_+) := -\overline{a}(u_-, u_+)\,(U(u_+) - U(u_-)) + F(u_+) - F(u_-).$$

The entropy inequality (2.3) holds on a shock wave from u_- to u_+ if and only if

$$E(u_-, u_+) \le 0. \tag{2.4}$$

Moreover, classical shocks satisfy (2.4).

As in [17], we define the **tangent function** $\varphi^\natural : \boldsymbol{R} \to \boldsymbol{R}$ associated with the flux f by $\varphi^\natural(u) = u$ if and only if $u = 0$, and

$$f'(\varphi^\natural(u)) = \frac{f(u) - f\big(\varphi^\natural(u)\big)}{u - \varphi^\natural(u)}, \quad \text{and } \varphi^\natural(u) \ne u \quad \text{for } u \ne 0.$$

Additionally, we define the **zero entropy dissipation function** $\varphi_0^\flat : \boldsymbol{R} \mapsto \boldsymbol{R}$ by

$$E(u, \varphi_0^\flat(u)) = 0 \quad \text{and } \varphi_0^\flat(u) \ne u \quad \text{for } u \ne 0.$$

It can be checked that

$$(\varphi_0^\flat \circ \varphi_0^\flat)(u) = u, \qquad u \in \boldsymbol{R}. \tag{2.5}$$

3. The Nonclassical Solver and the Nucleation Solver

In this section, we present a nonclassical Riemann solver that is different from the one in [17] in that it sometimes substitutes a classical solution where the earlier solver used a nonclassical solution. The substitution is based on a new ingredient, the "nucleation condition". The **Riemann problem** is the initial value problem for equation (2.1), in which the initial data are two constants:

$$u(x,0) = \begin{cases} u_l, & x < 0, \\ u_r, & x > 0. \end{cases} \tag{3.1}$$

Imposing the single entropy inequality (2.3) already restricts the class of admissible solutions. Only one free parameter remains to be determined, and the range of nonclassical shocks is constrained by the zero-entropy dissipation function $\varphi_0^\flat$ defined above. Therefore, as in [17], we supplement the Riemann problem with an additional selection criterion called a **kinetic relation.**

Let $\varphi^\flat : \boldsymbol{R} \mapsto \boldsymbol{R}$ be a **kinetic function**, i.e., by definition, a monotone decreasing and Lipschitz continuous mapping such that

$$\begin{aligned} &\varphi_0^\flat(u) < \varphi^\flat(u) \le \varphi^\natural(u), \quad u > 0, \\ &\varphi^\natural(u) \le \varphi^\flat(u) < \varphi_0^\flat(u), \quad u < 0, \end{aligned} \tag{3.2}$$

The kinetic function will be applied to select nonclassical shock waves. Observe that (2.5) and (3.2) imply the following **contraction property**:

$$|\varphi^\flat\big(\varphi^\flat(u)\big)| < |u|, \quad u \ne 0. \tag{3.3}$$

From $\varphi^\flat$ we also define its companion function $\varphi^\sharp : \boldsymbol{R} \to \boldsymbol{R}$ as follows: $\varphi^\sharp(u) = \varphi^\flat(u)$ if $\varphi^\flat(u) = \varphi^\natural(u)$; otherwise $\varphi^\sharp(u) \ne \varphi^\flat(u) \ne u$ is specified by

$$\frac{f(u) - f\big(\varphi^\sharp(u)\big)}{u - \varphi^\sharp(u)} = \frac{f(u) - f\big(\varphi^\flat(u)\big)}{u - \varphi^\flat(u)}, \quad u \ne 0. \tag{3.4}$$

Similarly, from the zero-dissipation function $\varphi_0^\flat$ we define $\varphi_0^\sharp : \boldsymbol{R} \to \boldsymbol{R}$ by replacing $\varphi^\flat$ by $\varphi_0^\flat$ in (3.4). By (3.2), we have

$$\begin{aligned} \varphi^\natural(u) \le \varphi^\sharp(u) < \varphi_0^\sharp(u), \quad u > 0, \\ \varphi_0^\sharp(u) < \varphi^\sharp(u) \le \varphi^\natural(u), \quad u < 0. \end{aligned}$$

Now we specify all the shock waves that we *temporarily* deem **admissible**, namely

- all classical shocks, together with
- all nonclassical shocks connecting states u_-, u_+ satisfying the **kinetic relation**

$$u_+ = \varphi^\flat(u_-). \tag{3.5}$$

Restricting attention to admissible shock waves and rarefaction waves only, the Riemann problem admits fewer solutions than under the entropy inequality alone, but there are still *two solutions* for every choice of $u_r < \varphi^\sharp(u_l)$ if $u_l > 0$ (and for every $u_r > \varphi^\sharp(u_l)$ if $u_l < 0$), provided $\varphi^\flat(u_l) \neq \varphi^\natural(u_l)$. For definiteness, consider a positive left-hand state $u_l > 0$. One solution is classical: it consists of either a single shock (if $u_r > \varphi^\natural(u_l)$), or a pattern made of a (right-characteristic) shock followed by a rarefaction (if $u_r < \varphi^\natural(u_l)$). The other solution is non-classical: it consists of an nonclassical shock from u_l to $\varphi^\flat(u_l)$ and a faster wave from $\varphi^\flat(u_l)$ to u_r, either a classical shock (if $u_r > \varphi^\flat(u_l)$), or a rarefaction (if $u_r < \varphi^\flat(u_l)$).

The Nucleation Criterion.

To select a unique solution of the Riemann problem (for given initial data u_l, u_r for which there are two solutions satisfying the entropy inequality (2.3) and the kinetic relation (3.5)), we need to introduce a **selection rule.** In principle, the selection rule could take the following abstract form: for each u_l there corresponds a set $\mathcal{N}(u_l)$, with

$$\mathcal{N}(u_l) \subset \{u < \varphi^\sharp(u_l)\} \text{ if } u_l > 0, \quad \mathcal{N}(u_l) \subset \{u > \varphi^\sharp(u_l)\} \text{ if } u_l < 0,$$

and $\mathcal{N}(0) := \emptyset$. The selection rule would then be :

$$\begin{aligned} &\textbf{If } u_r \in \mathcal{N}(u_l)\textbf{, then the solution is nonclassical;} \\ &\textbf{otherwise, the solution is classical.} \end{aligned} \tag{3.6}$$

For example, with the choice $\mathcal{N}(u_l) = \emptyset$ we take the classical solution for all u_r (for this value of u_l). At the other extreme, if $\mathcal{N}(u_l) := \{u < \varphi^\sharp(u_l)\}$, then we recover the solution specified in [17]; this latter rule selects the nonclassical solution whenever it is available.

A simple selection rule that we call the **nucleation condition** is to define the set $\mathcal{N}(u_l)$ through a threshold. Specifically, we consider a Lipschitz continuous **nucleation threshold function** $\varphi^N : \boldsymbol{R} \to \boldsymbol{R}$ with the property

$$\begin{aligned} \varphi^\natural(u) \le \varphi^N(u) \le \varphi^\sharp(u), \quad u > 0, \\ \varphi^\sharp(u) \le \varphi^N(u) \le \varphi^\natural(u), \quad u < 0. \end{aligned} \tag{3.7}$$

We then define the **nonclassical set**

$$\mathcal{N}(u_l) := \begin{cases} [\varphi^N(u_l), +\infty), & u_l < 0, \\ (-\infty, \varphi^N(u_l)], & u_l > 0. \end{cases} \tag{3.8}$$

In conclusion, we define :

Definition 3.1. *Consider a kinetic function and a nucleation threshold satisfying* (3.2) *and* (3.7)*. The* **Riemann solver with kinetics and nucleation** *is the solution of the Riemann problem with data* u_l, u_r *that satisfies the entropy inequality* (2.3)*, the kinetic relation* (3.5)*, and the nucleation criterion* (3.6)*,* (3.8)*. For brevity, we refer to this Riemann solver as the* **nucleation solver.** *(It is shown graphically in Figure 3.1.)*

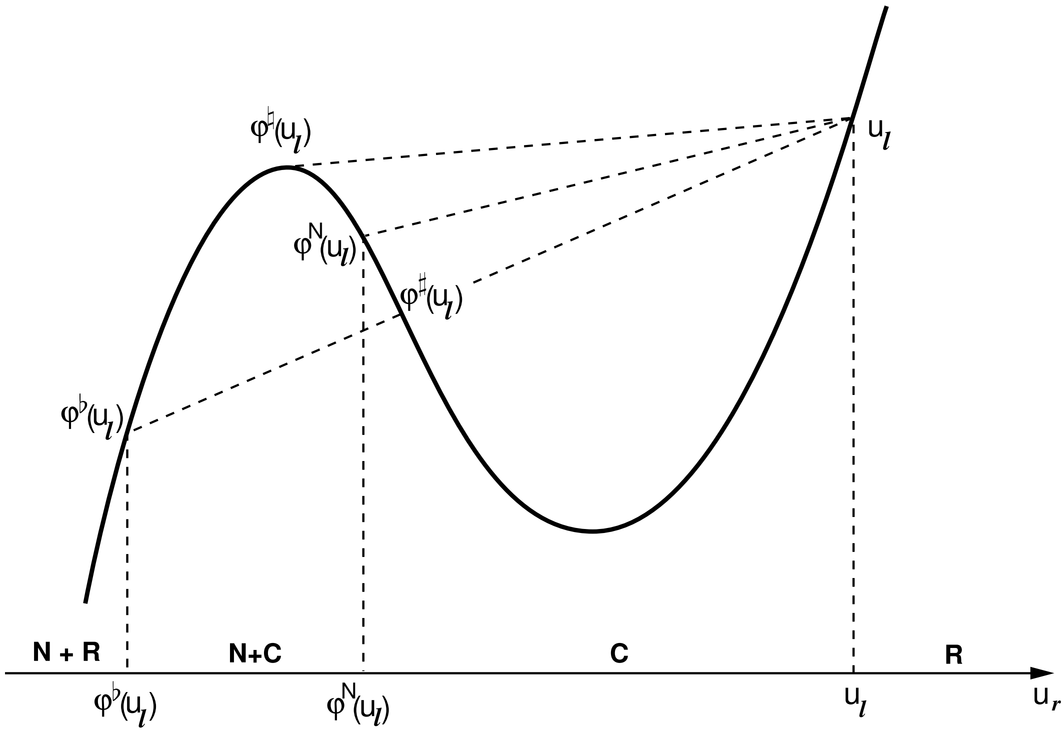


Fig. 3.1: Solution of the Riemann Problem using the Nucleation Solver.
C: Classical shock; **R:** Rarefaction; **N:** Nonclassical shock.

It will be convenient to define the set of admissible shocks to be those that appear in solutions of the Riemann solver with kinetics and nucleation. That is:

Definition 3.2. *For a given* $u_- > 0$ *a classical shock from* u_- *to* u_+ *is said to be* **admissible** *if and only if* $u_+ \geq \varphi^N(u_-)$ *and, similarly if* $u_- < 0$*, the classical shock is admissible if and only if* $u_+ \leq \varphi^N(u_-)$*. All nonclassical shocks satisfying the kinetic relation are* **admissible***.*

It is worth emphasizing that the Riemann solver with kinetics and nucleation is not uniquely characterized by the family of admissible waves, consisting of rarefactions and admissible shocks. Indeed, we show with examples that some Riemann problems have *two solutions* that can both be constructed from admissible shocks; only one of them is selected by the nucleation solver. Interestingly enough, as will be clarified in the following section, the second solution is significant for the theory, since it can appear as the asymptotic solution for large time.

It is also worth pointing out that the solution of the Riemann problem with nucleation is *not continuous in* L^1 with respect to the initial data, unless $\varphi^N \equiv \varphi^\sharp$. Again, this will be illustrated shortly with examples.

Remark 3.3. 1) If the restriction $\varphi^\natural(u) \le \varphi^N(u)$ is relaxed to allow $\varphi^N(u_l) < \varphi^\natural(u_l)$, then the transition from classical to nonclassical solution takes place with a shock-rarefaction giving way to a nonclassical shock-classical shock structure. This makes analysis of wave interactions more complicated, so we adopt the restriction (3.7) for simplicity.

2) No "natural" choice can be made for the solution of the Riemann problem with data u_l and $u_r = \varphi^N(u_l)$. Indeed, it is not difficult to see that by approaching the Riemann data with suitably constructed sequences of initial data one can approach both the (classical) one-wave and the (nonclassical) two-wave solutions of this Riemann problem. Modulo minor changes, all of the conclusions in the present paper remain valid if one replaces the nonclassical set in (3.8) by the *open* set:

$$\mathcal{N}(u_l) = \begin{cases} \big(\varphi^N(u_l), +\infty\big), & u_l < 0, \\ \big(-\infty, \varphi^N(u_l)\big), & u_l > 0. \end{cases}$$

4. The Cauchy problem

In this section we prove the existence of solutions for the Cauchy problem

$$\begin{aligned} &\partial_t u + \partial_x f(u) = 0, \qquad && u = u(x,t) \in \boldsymbol{R},\ x \in \boldsymbol{R},\ t > 0, \\ &u(x,0) = u_0(x), && x \in \boldsymbol{R}, \end{aligned} \tag{4.1}$$

by constructing approximate solutions by Dafermos' wave front tracking scheme [9, 17, 14].

Let $u_0 : \boldsymbol{R} \to \boldsymbol{R}$ be a function with bounded variation and for (small) $h > 0$, let u_0^h be a piecewise constant approximation of u_0 that has finitely many jumps and satisfies the uniform bounds

$$\begin{aligned} &\inf u_0 \le u_0^h \le \sup u_0, \\ &TV(u_0^h) \le TV(u_0), \\ &u_0^h \to u_0 \ \text{ in } L^1_{\text{loc}}, \text{ as } h \to 0. \end{aligned} \tag{4.2}$$

At each jump point x of u_0^h, solve (at least locally in time) the Riemann problem associated with the initial data $u_0^h(x\pm)$, by using the nucleation solver described in Section 3.

As is usual, rarefaction fans are decomposed into small rarefaction-fronts (i.e., expansion-shocks) with small strength, less than h. Each small jump travels with the speed determined by the Rankine-Hugoniot relation. Patching together these local solutions we obtain the approximate solution $u^h = u^h(x,t)$ defined up to the first interaction time t_1 when two waves from different Riemann solutions meet. At each wave interaction, we have a Riemann problem, which is solved by using the nucleation solver of Section 3, decomposing the jump into propagating fronts. Here, contrary to what is done at the initial time, we simply replace any outgoing rarefaction fan by a single rarefaction-front traveling with the Rankine-Hugoniot speed. Hence, there are at most two outgoing waves in each Riemann solution, so that the total number of waves remains bounded. Under suitable conditions, specified in detail just below, the argument in [17] establishes that the number of wave interactions is also finite; consequently $u^h(x,t)$ is defined for all (x,t).

In addition to the set of assumptions already put forward in Section 2, we also assume that the Lipschitz constant of $\varphi^\flat \circ \varphi^\flat$ near $u = 0$ is strictly less than 1,

$$\limsup_{\substack{u,v \to 0, \\ u \ne v}} \left| \frac{\varphi^\flat \circ \varphi^\flat(v) - \varphi^\flat \circ \varphi^\flat(u)}{v - u} \right| < 1, \tag{4.3}$$

and that the companion function $\varphi^\sharp : \boldsymbol{R} \to \boldsymbol{R}$ associated with the kinetic function $\varphi^\flat$ satisfies

$$u\,\varphi^\sharp(u) \le 0, \quad u \in \boldsymbol{R}. \tag{4.4}$$

Condition (4.4) implies that the Riemann solution is always classical when the Riemann data are in the same region of convexity or concavity of f. (All of these assumptions are fulfilled in most situations of interest; see [17].)

The following theorem establishes the existence of a solution of the Cauchy problem, defined using the nucleation solver. It will be convenient to introduce the notation $u(t)$ for the function $x \mapsto u(x,t)$.

Theorem 4.1. *Consider the Cauchy problem* (4.1) *for the conservation law associated with a concave-convex flux-function f satisfying* (2.2)*. Consider a kinetic function $\varphi^\flat$ satisfying the assumptions* (3.2)*,* (4.3)*, and* (4.4)*, and a threshold nucleation function φ^N satisfying* (3.7)*.*

(i) *Then, for arbitrary initial data $u_0 \in BV(\boldsymbol{R})$, the wave front tracking approximations determined from the nonclassical Riemann solver satisfy, for some constants $C_1, C_2 > 0$ depending only on $\|u_0\|_{L^\infty(\boldsymbol{R})}$ and on the data f and $\varphi^\flat$,*

$$\begin{aligned} &(a) \quad \|u^h(t)\|_{L^\infty(\boldsymbol{R})} \le C_1, \\ &(b) \quad TV(u^h(t)) \le C_2\, TV(u_0), \\ &(c) \quad \|u^h(t) - u^h(s)\|_{L^1(\boldsymbol{R})} \le C_2\, TV(u_0)\, \sup_{|w|\le C_1} |f'(w)|\, |t-s|, \end{aligned} \tag{4.5}$$

for all $s, t \ge 0$.

(ii) *A subsequence of u^h converges strongly in L^1_{loc} to a weak solution $u = u(x,t)$ of the Cauchy problem* (4.1)*, with*

$$\begin{aligned} &(a) \quad \|u(t)\|_{L^\infty(\boldsymbol{R})} \le C_1, && t \ge 0, \\ &(b) \quad TV(u(t)) \le C_2\, TV(u_0), && t \ge 0, \\ &(c) \quad \|u(t_2) - u(t_1)\|_{L^1(\boldsymbol{R})} \le C_2\, TV(u_0)\, \sup_{|w|\le C_1} |f'|\, |t_2 - t_1|, && t_1, t_2 \ge 0. \end{aligned} \tag{4.6}$$

(iii) *In addition, the solution u satisfies the entropy inequality*

$$\partial_t U(u) + \partial_x F(u) \le 0. \tag{4.7}$$

Proof. The proof is virtually identical to the one given in [3,17]. The only difference comes in the choice of the Riemann solver, which is taken here to be the nucleation solver described in Section 3. The proof is based on a careful analysis of interaction cases. The novelty here is that several interaction cases are now solved with the classical Riemann solution rather than with the nonclassical one. Modulo this, all the arguments of proof go through. See [17, Section IV-3]. □

Based on Theorem 4.1 we can now define a solution operator, providing us with the **nonclassical solutions with nucleation** at time t, by

$$S_t u_0 := \lim_{h\to 0} u^h(x,t), \tag{4.8}$$

in which u^h is the wave-tracking solution associated with *a specific* sequence of initial data u_0^h. By Theorem 4.1 the limit in (4.8) exists, at least for a *subsequence* $h \to 0$.

Some important remarks should be made on the solution operator S_t. Since we do not have a uniqueness result (and we do not expect the solutions to be unique), the operator S_t need not be a semi-group. Modifying the subsequence $h \to 0$ or choosing another sequence of initial data u_0^h may generate a *different* solution $S_t u_0$. Strictly speaking, S_t does not depend upon u_0 only, but on the approximations u_0^h and the subsequence $h \to 0$ as well.

When no nucleation is allowed, that is when $\varphi^N \equiv \varphi^\sharp$, it is conjectured in [17] that the solutions constructed in Theorem 4.1 are uniquely determined by their initial data. More precisely, S_t is expected to be an L^1-Lipschitz continuous, semi-group of solutions, satisfying therefore

$$S_t \circ S_s = S_{t+s}, \qquad t, s \geq 0, \tag{4.9}$$

and

$$\|S_t u_0 - S_s u_0\|_{L^1(\boldsymbol{R})} \leq C\left(\|v_0 - u_0\|_{L^1(\boldsymbol{R})} + |t - s|\right). \tag{4.10}$$

When $\varphi^N \neq \varphi^\sharp$ both properties (4.9) and (4.10) no longer hold for the solution-operator generated from the solver with nucleation. To see that the solution operator is not continuous with respect to its initial data, consider the sequence of initial data

$$u_0^\eta(x) = \begin{cases} u_*, & x < 0, \\ \varphi^N(u_*) + \eta, & x > 0, \end{cases}$$

where $u_* > 0$ is a point where $\varphi^N(u_*) < \varphi^\sharp(u_*)$. We have

$$\lim_{\eta \to 0} \|u_0^\eta - u_0^{-\eta}\|_{L^1(\boldsymbol{R})} = 0,$$

but the corresponding solution at any time $t > 0$ is a single shock if $\eta > 0$ but a two wave pattern if $\eta < 0$ and therefore

$$\lim_{\eta \to 0} \|S_t u_0^\eta - S_t u_0^{-\eta}\|_{L^1(\boldsymbol{R})} > 0.$$

Theorem 4.1 applies, in particular, to initial data which are perturbations of Riemann data:

$$\lim_{x \to -\infty} u_0(x) = u_l, \qquad \lim_{x \to +\infty} u_0(x) = u_r,$$

where u_l, u_r are given. Solutions generated by wave-front tracking satisfy the property of propagation with finite speed and it can be checked that

$$\lim_{x \to -\infty} (S_t u_0)(x) = u_l, \qquad \lim_{x \to +\infty} (S_t u_0)(x) = u_r$$

for all times t. As already pointed out at the end of Section 3, in some range for the data u_l and u_r the Riemann problem can be solved using admissible waves with two different patterns: a single shock wave, or a two-wave pattern. Let us refer here to these two solutions as w_1 and w_2.

Heuristically, when the Riemann data are within the range where two solutions exist, we expect the solution $S_t u_0$ to converge asymptotically in time toward one of these two admissible Riemann solutions. Introducing the similarity variable $\xi = x/t$, we define

$$w(\xi) := \lim_{t \mapsto \infty} (S_t u_0)(\xi\, t),$$

assuming that this limit exists.

A significant open problem is to determine conditions on the initial data (or rather conditions on the sequence of initial data u_0^h) which would ensure that w coincide with one of the two solutions w_1 and w_2. That is, to determine the domains of attraction of the asymptotic solutions w_1, w_2. It seems that no simple criterion is available. For instance, a condition on the amplitude of the initial data would not be sufficient, as waves can be cancelled out. In Examples 4.2 to 4.4 below, we illustrate the difficulties with simple piecewise constant initial data.

Example 4.2. **Two possible time-asymptotic behaviors.**

In this example, we specify two choices of piecewise constant initial data

$$u(x,0) = u_0^{(j)}(x),$$

for which the solution using wave front tracking has different asymptotic behavior as $t \to +\infty$, even though the initial data have the same limits $u_\pm$ as $x \to \pm\infty$. The conclusion from this example is that solutions of the Cauchy problem need not converge to the solution singled out by the nucleation solver with initial data $u_\pm$.

Let $u_l > 0$, and let $u_r \in (\varphi^N(u_l), \varphi^\sharp(u_l))$. Thus the solution of the Riemann problem given by the nucleation solver is a single classical shock from u_l to u_r. Now let $u_m^{(1)} \in (\varphi^\natural(u_l), \varphi^N(u_l))$ and let $u_m^{(2)} \in (\varphi^N(u_l), u_r)$. Then we define initial data

$$u_0^{(j)}(x) := \begin{cases} u_l, & x < 0, \\ u_m^{(j)}, & 0 < x < 1, \\ u_r, & x > 1. \end{cases}$$

The solutions with these choices of initial data are shown in Figure 4.1. In the figure, the waves are labeled N for nonclassical shock, C for classical shock and R for rarefaction. The arrows indicate whether the solution u is increasing or decreasing from left to right across the wave. The asymptotic behavior of the solutions as $t \to \infty$ is quite different: the corresponding solution $u^{(1)}$ and $u^{(2)}$ having exactly one wave and two waves respectively.

Example 4.3. **The order in which waves interact does matter.**

One might speculate that the regions of attraction of the two attractors identified in Example 4.2 could be characterized by a simple threshold condition on the range of the initial data, saying roughly speaking that, under small perturbations, a single classical shock would split into a two wave structure if and only if the perturbation exceeds some threshold. In this example, we show that a threshold is not available, leading us to conclude that the boundary between regions of attraction may be quite complex.

Consider initial data $u(x,0) = u_0(x)$ shown in Figure 4.2:

$$u_0(x) = \begin{cases} u_l, & x < 0, \\ u_1, & 0 < x < a, \\ u_2, & a < x < b, \\ u_r, & x > b, \end{cases}$$

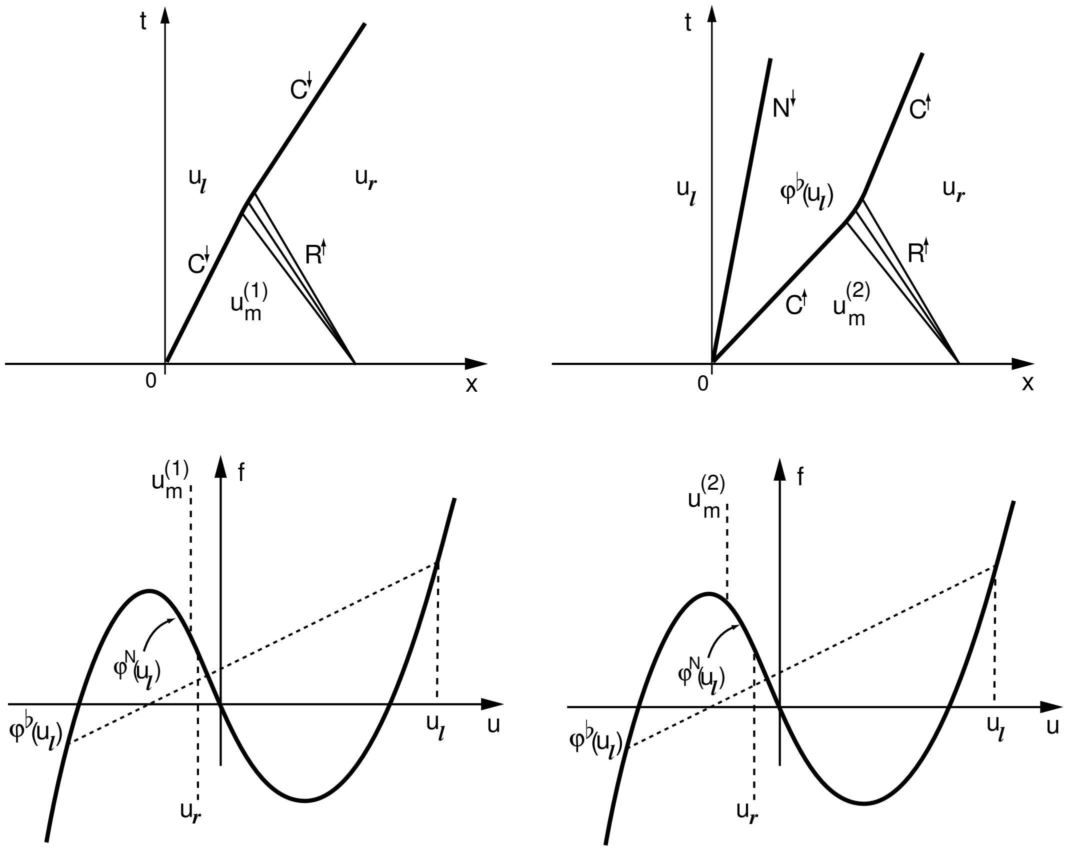


Figure 4.1: Two possible time-asymptotic behaviors (Example 4.2).

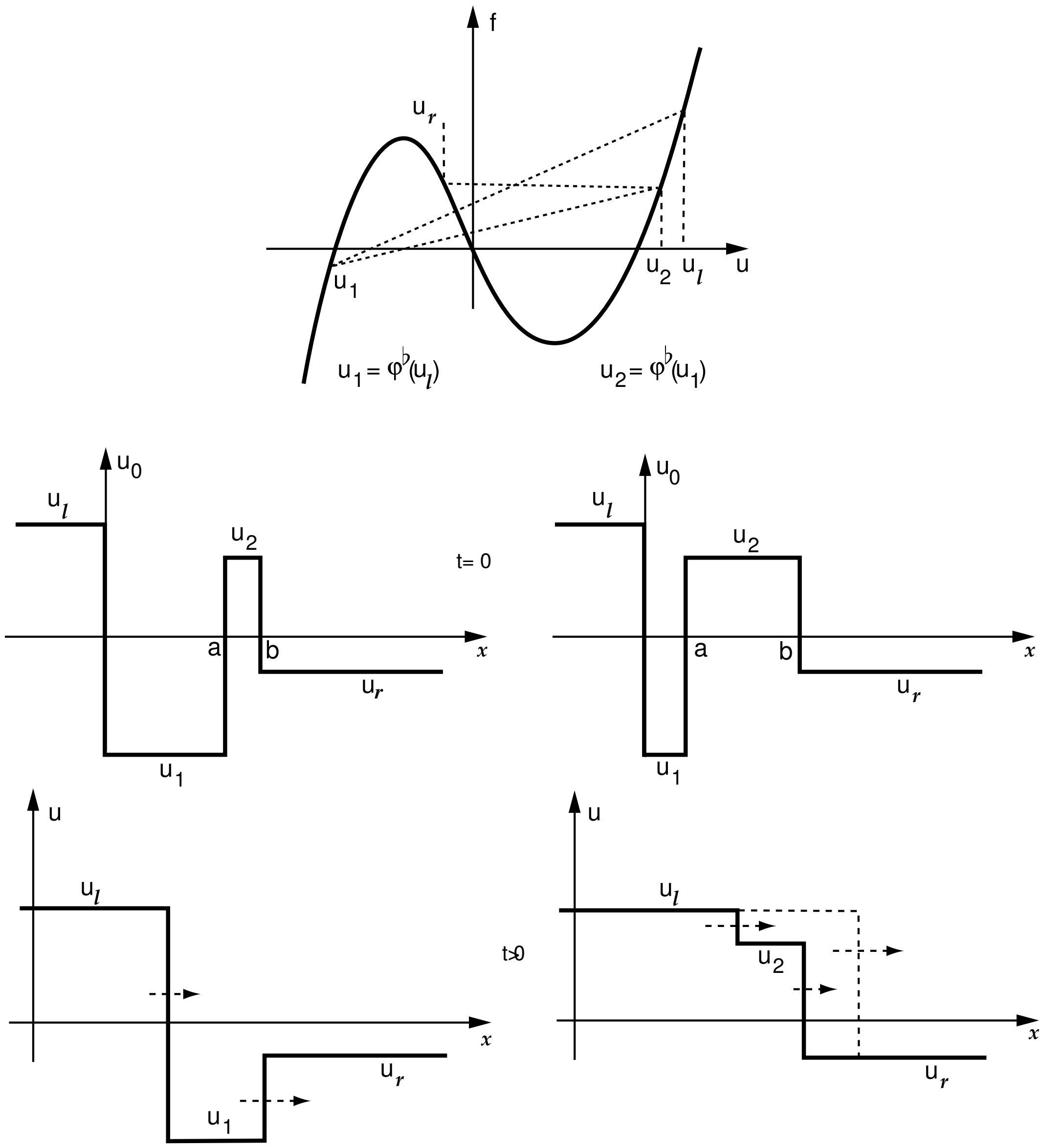
in which $u_1 = \varphi^\flat(u_l)$ and $u_2 = \varphi^\flat(u_1)$. (These seemingly special relationships between the intermediate states merely simplify the solution; nearby choices for u_1, u_2 give rise to further wave interactions, but otherwise the structure of the solution is the same.) In order to have the possibility of no nonclassical shocks in the long-time behavior, we let u_r satisfy $\varphi^N(u_l) < u_r < \varphi^\sharp(u_l)$.

The spacing defined by the locations a and b controls the subsequent motion. If a is large compared to $b - a$, then the nonclassical waves are spaced far apart, and the slower wave will first catch up to the classical shock from u_2 to u_r. The result, shown in Figure 4.3, is a fast classical shock from u_1 to u_r, which moves ahead of the nonclassical shock from u_l to u_1.

When a is small compared with $b-a$, then the nonclassical wave from u_l to u_1 collides with the slower one from u_1 to u_2, before the latter wave can catch up to the classical compressive shock from u_2 to u_r. The result of the interaction between these two nonclassical waves is simple cancellation, leaving a fast compressive shock. This shock then quickly overtakes the classical shock from u_2 to u_r, leaving only the classical shock from u_l to u_r. This illustrated in Figure 4.2. Thus, although u_1 is well below the nucleation threshold $\varphi^N(u_l)$, nonetheless the asymptotic solution need not contain any nonclassical shocks.

Example 4.4. **Splitting/merging solutions.**

In this example, we demonstrate the splitting of a classical shock into a nonclassical shock



(i) a large, $b - a$ small. (ii) a small, $b - a$ large.

Figure 4.2: The order in which waves interact does matter (Example 4.3).

and a classical shock, and then the merging of this structure back into a classical shock. In the next section we give a theoretical treatment for general initial data near that of the example, showing repeated splitting and merging.

Consider initial data of the following form (see Figure 4.3).

$$u_0(x) = \begin{cases} u_l, & x < 0, \\ u_1, & 0 < x < a, \\ u_2, & a < x < b, \\ u_r, & x > b. \end{cases}$$

We assume $u_l > 0$, and the following inequalities:

$$\varphi^\flat(u_l) < u_2 < \varphi^N(u_l) < u_1 < \varphi^\sharp(u_l) < u_r < \varphi^N(\varphi^\flat(u_l)) < u_l.$$

Now the solution of the Riemann problem with data u_1, u_2 is a rarefaction wave, which will interact quickly (if a is small) with the classical shock from u_l to u_1. To simplify this interaction, we replace (as in wave front tracking) the rarefaction by an expansion shock from u_1 to u_2. With this observation, the solution of the initial value problem is shown in Figure 4.4, assuming that a is small compared with $b - a$.

The first interaction results in a pair of shocks, a nonclassical shock $N^\downarrow$ and a classical shock $C^\uparrow$. (Recall from Example 4.2 that the arrows are a convenient way to record whether u is increasing or decreasing across the shock from left to right.) Subsequently, a shock approaches from the right, and slows down the $C^\uparrow$ to a speed that is below that of the $N^\downarrow$ shock to the left, resulting in the final merging.

In the analysis of the next section, we take $\varphi^N(u_l)$ close to $\varphi^\sharp(u_l)$, so that the construction makes sense when u_1, u_2, u_r are all close. Then the main features of Figure 4.3 are big shocks, either $N^\downarrow$ or $C^\uparrow$, from $\varphi^\flat(u_l)$ to one of u_2 or u_r, and $C^\downarrow$, from u_l to u_1 or u_r. The analysis will show how this basic structure of big waves and small waves is maintained when the big wave structure is perturbed slightly.

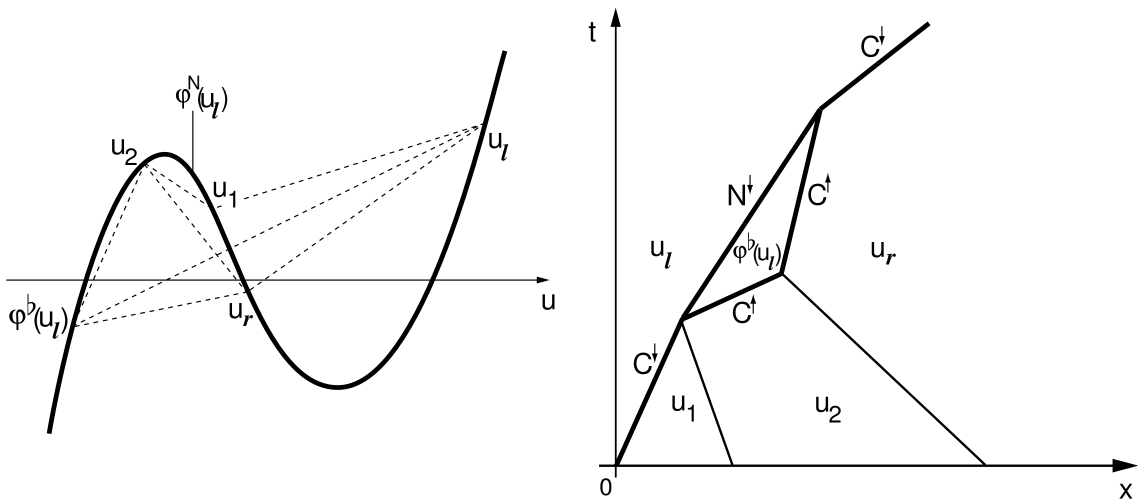


Figure 4.3: Splitting/merging solutions (Example 4.4).

5. A Class of Splitting/Merging Solutions

In this section, generalizing Example 4.4, we establish the existence of a large class of solutions whose structure, illustrated in Figure 5.1, consists of large shocks (one or two at each time t) undergoing repeated splitting and merging. The large waves separate regions in the $(x, t)-$ plane where the solution has small and decaying total variation. Interestingly enough, we will see that the splitting/merging feature can take place infinitely many times when $\varphi^N \equiv \varphi^\sharp$ but *only finitely many times* when a nucleation criterion is acting.

We restrict attention to initial data having a specific structure that we now describe. Given $u_* > 0$, we consider initial data $u(x, 0) = u_0(x)$ of the form

$$u_0(x) = u_0^N(x) + v_0(x), \tag{5.1}$$

where

$$u_0^N(x) := \begin{cases} u_*, & x < 0, \\ \varphi^N(u_*), & x > 0, \end{cases}$$

and $v_0 : \boldsymbol{R} \to \boldsymbol{R}$ has small total variation:

$$TV(v_0) < \epsilon. \tag{5.2}$$

In addition to the size of the perturbation ϵ, we have another parameter in the problem

$$\eta := \varphi^\sharp(u_*) - \varphi^N(u_*), \tag{5.3}$$

which we also assume to be small. Note that u_0^N is a single step function which admits two distinct Riemann solutions made of admissible waves.

If the perturbation v_0 were chosen to be a single step (located at $x = 0$), connecting 0 to δ (with δ sufficiently small) then the solution of the corresponding initial value problem depends on the sign of δ :

- For $\delta > 0$, the Riemann solution is a single classical shock $C^\downarrow$:

$$u^\downarrow(x, t) := \begin{cases} u_*, & x < s\,t, \\ \varphi^N(u_*) + \delta, & x > s\,t, \end{cases} \tag{5.4}$$

  in which $s := \overline{a}(u_*, \varphi^N(u_\ell) + \delta)$;
- For $\delta < 0$, we get a two-wave solution $u^{\downarrow\uparrow}(x, t)$ consisting of an nonclassical shock $N^\downarrow$ from u_* to $\varphi^\flat(u_*)$ plus a faster classical shock $C^\uparrow$ from $\varphi^\flat(u_*)$ to $\varphi^N(u_*) - \delta$.

We are going to exhibit a certain structure for the solution of the initial value problem (4.1), (5.1), in which these two solutions of the Riemann problem play a dominant role. Specifically, we will find (illustrated in Figure 5.1) a solution with either one or two big waves at each time $t > 0$. When there is a single wave, it is a perturbation of the solution $u^\downarrow$, and when there are two waves, the solution is a perturbation of $u^{\downarrow\uparrow}$.

If we further assume $\varphi^N(u) < \varphi^\sharp(u)$, i.e., that the nucleation condition does not coincide with the kinetic relation, then we show there are a finite number of *splittings*, in which $C^\downarrow$ gives way to $N^\downarrow$ and $C^\uparrow$, and corresponding *mergings,* in which $N^\downarrow$ and $C^\uparrow$ interact (i.e., meet), resulting in $C^\downarrow$. Thus, the long-time behavior of the solution, with either one or two big waves, is achieved after a finite time. As for classical entropy solutions (Dafermos [10]), the small perturbations in the solution not represented by these big waves decay in time, so that the solution approaches a piecewise constant function of x as $t \to +\infty$.

In Figure 5.1, we identify the locus of big shocks $N^{\downarrow}$ and $C^{\downarrow}$ as a curve $x = y(t)$, and the locus of the big shock $C^{\uparrow}$ by $x = z(t)$. Observe that the curve $z(t)$ is defined only for those times t when the solution has a double-wave structure. Away from these curves, the solution is expected to have small total variation (of order ϵ). In the following, a function having this structure will be called a **splitting/merging solution.**

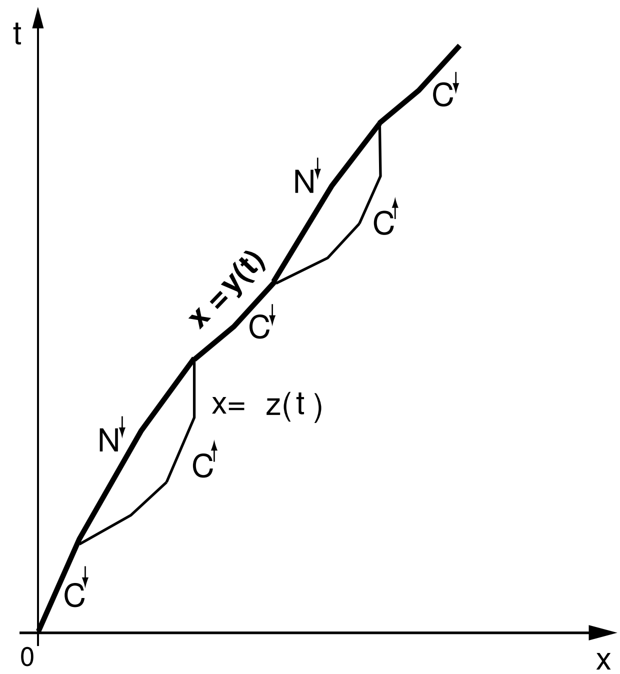


Figure 5.1: Splitting/merging solution.

For the analysis, we introduce the notion of *generalized strength* (which extends that of [17]). It is based upon redefining the strength of nonclassical shocks via a Lipschitz continuous function $\psi : \boldsymbol{R} \mapsto \boldsymbol{R}$ satisfying

$$\begin{aligned} \varphi^N(u) \le \psi(u) \le \varphi^\sharp(u), \quad u > 0, \\ \varphi^\sharp(u) \le \psi(u) \le \varphi^N(u), \quad u < 0. \end{aligned} \tag{5.5}$$

A first attempt is to define the generalized strength of the nonclassical shock connecting u to $\varphi^\flat(u)$ (with $u > 0$, for instance) to be

$$\sigma^\psi(u) := (u - \psi(u)) - (\psi(u) - \varphi^\flat(u)). \tag{5.6}$$

When $\varphi^N \equiv \varphi^\sharp$, this choice ensures that the strengths are *continuous* (up to perturbation due to small waves) when the two large waves combine together or when a classical shock splits; see [17, Remarks VIII-1.2]. More generally, when $\varphi^N \neq \varphi^\sharp$, (5.6) ensures that the strengths are *decreasing* at mergings and splittings. The formula (5.6) needs to be modifed, as we now discuss.

First, to see the role of the range of ψ, consider the two extreme choices:

$$\sigma^\sharp := \sigma^{\varphi^\sharp}, \quad \sigma^N := \sigma^{\varphi^N}.$$

Since σ^ψ is linear and decreasing with respect to ψ, we have the following property:

$$\sigma^\sharp(u) \le \sigma^\psi(u) \le \sigma^N(u) \quad \text{for all } u > 0.$$

Thus, in order that the generalized strength be positive, no matter the choice of $\psi(u) \in [\varphi^N(u), \varphi^\sharp(u)]$, we would need to assume :

$$u - \varphi^\sharp(u) > \varphi^\sharp(u) - \varphi^\flat(u), \quad u > 0. \tag{5.7}$$

Inequality (5.7) is satisfied if $\varphi^\flat(u) > -u$ and $\varphi^\sharp(u) < 0$. For example, this is true for all $u > 0$ if f is an odd function and the entropy function is $U(u) = u^2/2$. Similarly, these inequalities are satisfied for u near zero. (See Chapter VIII in [17].)

To cover general flux-functions and kinetic functions beyond those satisfying (5.7), we also modify the strength of the big, increasing classical shock $C^\uparrow$ located at $z = z(t)$ (when it exists in the solution). If $C^\uparrow$ connects states u_-, u_+ say, we define its strength as $\varphi^\flat(u_-) - \varphi^\flat(u_+) > 0$. Then, instead of (5.6) we set

$$\sigma^\psi(u) := (u - \psi(u)) - (\varphi^\flat \circ \varphi^\flat(u) - \varphi^\flat \circ \psi(u)). \tag{5.8}$$

The continuity/decreasing properties mentioned above still hold. In addition, since for $u > 0$

$$\psi(u) < \varphi^\flat \circ \psi(u) < \varphi^\flat \circ \varphi^\flat(u) < u,$$

we also have :

Lemma 5.1. *The generalized strength $\sigma^\psi(u)$ defined in* (5.8) *is strictly positive.*

In defining the generalized total variation functional, we distinguish between the big waves and the (two or three) regions where the solution has small oscillations. Consider a piecewise constant, approximate, splitting/merging solution $u = u^h(x,t)$, associated with the shock curves $y = y^h(t)$ and $z = z^h(t)$. It is convenient to set $z^h(t) = y^h(t)$ when the solution contains a single shock. We define separately the total variation of small waves located to the left of the curve $y^h(t)$, between the two curves, and to the right of the curve $z^h(t)$

$$V^h_{\text{left}}(t) := TV_{-\infty}^{y^h(t)}(u^h(t)),$$

$$V^h_{\text{middle}}(t) := TV_{y^h(t)}^{z^h(t)}(u^h(t)),$$

and

$$V^h_{\text{right}}(t) := TV_{y^h(t)}^{+\infty}(u^h(t)).$$

We also set

$$V^h(t) = V^h_{\text{left}}(t) + \kappa_0\, V^h_{\text{middle}}(t) + \kappa_0\, V^h_{\text{right}}(t).$$

The strength of the big waves is determined by the functional $W^h(t)$, defined by

$$W^h(t) := \begin{cases} \sigma^\psi(u_-) + |\varphi^\flat \circ \tilde u_+ - \varphi^\flat \circ \tilde u_-|, & y^h(t) \text{ is a nonclassical shock,} \\ |u_+ - u_-|, & y^h(t) \text{ is a classical shock,} \end{cases} \tag{5.9}$$

where

$$u_\pm := \lim_{x \to y^h(t)\pm} u^h(x,t), \quad \tilde u_\pm := \lim_{x \to z^h(t)\pm} u^h(x,t),$$

Theorem 5.2. *Suppose that ϵ and η are sufficiently small and let us restrict attention to initial data of the form* (5.1), *satisfying* (5.2). *Then the piecewise constant approximate solutions $u^h = u^h(x,t)$ constructed from the nucleation solver have the splitting/merging structure described above. Moreover, for $\kappa_0, \kappa_1, \kappa_2 > 0$ sufficiently small and for each $t \geq 0$,*

$$V^h(t) + \kappa_2 W^h(t) \leq V^h(0) + \kappa_2 W^h(0), \tag{5.10}$$

and

$$\begin{aligned} &V^h_{\text{left}}(t) \leq V^h_{\text{left}}(0), \\ &V^h_{\text{right}}(t) \leq V^h_{\text{right}}(0), \\ &V^h_{\text{left}}(t) + \kappa_1 V^h_{\text{middle}}(t) \leq V^h_{\text{left}}(t) + \kappa_1 V^h_{\text{middle}}(t), \end{aligned} \tag{5.11}$$

At each splitting, the total variation $V^h(t) + \kappa_2 W^h(t)$ decreases by at least $\psi(u_*) - \varphi^N(u_*)$; at each merging it decreases by at least $\varphi^\sharp(u_*) - \psi(u_*)$.

Hence, if $\varphi^N(u_*) \neq \varphi^\sharp(u_*)$, then only finitely many mergings and splittings can take place and the (approximate) solution eventually settles to a solution having a specified one-wave or two-wave structure. In the absence of a nucleation criterion, i.e., when $\varphi^N(u_*) = \varphi^\sharp(u_*)$, the splittings and mergings may continue for all time.

By letting $h \to 0$, we obtain an exact solution $u = u(x,t)$ having the splitting/merging structure and composed of admissible waves only.

Remark 5.3. 1) More precisely, by taking ϵ arbitrary small, the decreasing amounts can be taken to be arbitrary close to $2\,(\psi(u_*) - \varphi^N(u_*))$ and $2\,(\varphi^\sharp(u_*) - \psi(u_*))$.

2) The total variation bounds, together with the standard property of propagation with finite speed, imply the L^∞ bounds

$$|u(x,t) - u_*| \leq V^h_{\text{left}}(t) \leq V^h_{\text{left}}(0) \leq \epsilon, \quad x < y^h(t),$$

$$|u(x,t) - \varphi^N(u_*)| \leq TV^{+\infty}_{z^h(t)}(u^h(t)) \leq (1+\kappa_1)\,\epsilon, \quad x > z^h(t),$$

$$|u(x,t) - \varphi^\flat(u_*)| \leq |\varphi^\flat(u(y^h(t)-,t)) - \varphi^\flat(u_*)| + TV^{z^h(t)}_{y^h(t)}(u^h(t)) \leq C\,\epsilon, \quad y^h(t) < x < z^h(t).$$

Proof. For simplicity, we remove the subscript h throughout the proof. Using the notation in [17] and in view of the list of interaction patterns given therein, we obtain the following :

• All interactions that do not involve the big waves located at $y^h(t)$ and $z^h(t)$ contain only classical waves. The standard total variation is non-increasing at each of these interactions.

• Consider a classical interaction $C^\uparrow$ involving the big increasing shock and a small wave. If u_l is connected to u_m by a big shock and u_m is connected to u_r by a small rarefaction or shock we have

$$\begin{aligned} \big[W(t)\big] &= |\varphi^\flat(u_r) - \varphi^\flat(u_l)| - |\varphi^\flat(u_m) - \varphi^\flat(u_l)| \\ &\leq Lip(\varphi^\flat)\,|u_r - u_m| \end{aligned}$$

and

$$\big[V_{\text{right}}(t)\big] = -|u_m - u_l|,$$

which implies that $\kappa_2 W(t) + V_{\text{right}}(t)$ is decreasing. The case where a small shock meets the big shock on the left is completely similar, replacing $V_{\text{right}}(t)$ by $V_{\text{left}}(t)$.

• The nonclassical wave exists in both the incoming and the outgoing pattern in only a limited family of interactions, classified as Cases RN and CN-3 in [17]. In this classification, the letters R,N, and C denote Rarefaction, Nonclassical shock, and Classical shock, respectively. It is easy to work out when a CN interaction involves both incoming and outgoing nonclassical waves; this is CN-3. The incoming wave strengths are $\sigma^\psi(u_m)$ and $|u_m - u_l|$ and the outgoing ones are $\sigma^\psi(u_l)$ and $|\varphi^\flat(u_l) - \varphi^\flat(u_m)|$. We find for the small waves

$$\begin{aligned}\big[V(t)\big] &= \kappa_0\,|\varphi^\flat(u_l) - \varphi^\flat(u_m)| - |u_m - u_l| \\ &\leq \big(\kappa_0\,Lip(\varphi^\flat) - 1\big)\,|u_m - u_l| < 0,\end{aligned}$$

and for the nonclassical wave

$$\big[W(t)\big] = \sigma^\psi(u_l) - \sigma^\psi(u_m) \leq Lip(\sigma^\psi)\,|u_m - u_l|.$$

Therefore $\big[V(t) + \kappa_2\,W(t)\big]$ is negative if

$$\kappa_0\,Lip(\varphi^\flat) + \kappa_2\,Lip(\sigma^\psi) < 1.$$

• The nonclassical shock in the incoming pattern is cancelled out by the big increasing classical shock in Case NC and the merge into a single big classical shock. The strength of small waves is unchanged. We have, since $\varphi^\flat(u_l) = u_m$,

$$\begin{aligned}\big[W(t)\big] &= (u_l - u_r) - \sigma^\psi(u_l) - (\varphi^\flat(u_m) - \varphi^\flat(u_r)) \\ &= (u_l - u_r) - (u_l - \psi(u_l)) - (\varphi^\flat \circ \psi(u_l) - \varphi^\flat \circ \varphi^\flat(u_l)) - (\varphi^\flat(u_m) - \varphi^\flat(u_r)) \\ &= -u_r + \varphi^\flat(u_r) + \psi(u_l) - \varphi^\flat \circ \psi(u_l).\end{aligned}$$

We find, since $\psi(u_l) < \varphi^\sharp(u_l) < u_r$ and $\varphi^\flat$ is monotonically decreasing,

$$\begin{aligned}\big[W(t)\big] &= -|\psi(u_l) - u_r| - |\varphi^\flat \circ \psi(u_l) - \varphi^\flat(u_r)| \\ &\leq -|\varphi^\sharp(u_l) - u_r| - |\varphi^\flat \circ \varphi^\sharp(u_l) - \varphi^\flat(u_r)| < 0.\end{aligned}$$

In addition, since u_l is close to u_* we have the following bound for the decrease:

$$\big[W(t)\big] \leq -(\varphi^\sharp(u_*) - \psi(u_*))/2.$$

• The nonclassical wave arises from the interaction in Case CR-4. For the small waves we find (as in [17])

$$\big[V(t)\big] = -\kappa_0\,(u_m - u_r) < 0$$

and for the big waves

$$\begin{aligned}\big[W(t)\big] &= \sigma^\psi(u_l) - (u_l - u_m) + (-\varphi^\flat(u_r) + \varphi^\flat \circ \varphi^\flat(u_l)) \\ &= (u_l - \psi(u_l)) + (\varphi^\flat \circ \psi(u_l) - \varphi^\flat \circ \varphi^\flat(u_l)) - (u_l - u_m) + (-\varphi^\flat(u_r) + \varphi^\flat \circ \varphi^\flat(u_l)) \\ &= -\psi(u_l) + u_m - \varphi^\flat(u_r) + \varphi^\flat \circ \psi(u_l).\end{aligned}$$

Hence,

$$\big[V(t)+\kappa_2\, W(t)\big] = -\kappa_0\,(u_m-u_r)+\kappa_2\,\big(-\psi(u_l)+u_m-\varphi^\flat(u_r)+\varphi^\flat\circ\psi(u_l)\big).$$

Observe that when $\kappa_0=\kappa_2=1$ and $\psi=\varphi^\sharp$ we find

$$\big[V(t)+\kappa_2\, W(t)\big] = -|\psi(u_l)-u_r| - |\varphi^\flat(u_r)-\varphi^\flat\circ\psi(u_l)| < 0.$$

More generally $\big[V(t)+\kappa_2\, W(t)\big]$ is negative if $\kappa_2\le\kappa_0$ and ψ is arbitrary within φ^N and $\varphi^\sharp$, since

$$\begin{aligned}\big[V(t)+\kappa_2\, W(t)\big] &= -\kappa_0\,(u_m-u_r)+\kappa_2\,\big(-\psi(u_l)+u_m-\varphi^\flat(u_r)+\varphi^\flat\circ\psi(u_l)\big)\\ &\le \kappa_2\,\Big(-u_m+u_r-\psi(u_l)+u_m-\varphi^\flat(u_r)+\varphi^\flat\circ\psi(u_l)\Big)\\ &= -\kappa_2\,\big(|\psi(u_l)-u_r|+|\varphi^\flat(u_r)-\varphi^\flat\circ\psi(u_l)|\big)\\ &\le -\kappa_2\,|\psi(u_l)-\varphi^N(u_l)|.\end{aligned}$$

In addition, since u_l is close to u_* we have

$$\big(\psi(u_l)-\varphi^N(u_l)\big) \ge (\psi(u_*)-\varphi^N(u_*))/2 > 0.$$

This completes the proof of Theorem 5.2. □

6. Application to Thin Liquid Films

The thin liquid film equation studied in [5] is

$$h_t+(h^2-h^3)_x = -(h^3h_{xxx})_x + D(h^3h_x)_x. \tag{6.1}$$

In this equation, $h=h(x,t)$ is the (nondimensionalized) height of a thin liquid film moving up an inclined flat solid surface. The nonconvex flux

$$f(h)=h^2-h^3,\quad 0<h<1,$$

contains the competing effects of gravity (the cubic contribution) and a surface stress known as the Marangoni stress, induced in experiments by an imposed constant thermal gradient along the solid surface. The fourth-order diffusion is supplied by surface tension, and the second-order diffusion, with a (small) nondimensional parameter D, represents a contribution of gravity to the pressure. The equation represents the lubrication approximation of two-dimensional Stokes flow with a free boundary.

Two kinds of numerical experiments were reported in [5], both setting $D=0$ in (6.1). In simulations of initial value problems, a downstream (precursor layer) height $h_r=0.1$ is fixed, and smooth initial data are chosen to approximate a sequence of Riemann problems, with upstream height $h_l>0.1$ being varied. In these simulations, both the single (classical) wave structure and the two wave structure with an undercompressive (nonclassical) wave are observed to emerge from the initial data. Moreover, both these structures can be observed for a range of choices of h_l, depending on the internal structure of the initial data. However, for all large enough h_l, roughly $h_l > 0.4$, only the two-wave structure emerges.

The other numerical experiments were carried out to explain the PDE results in terms of traveling waves approximating shocks. The traveling wave equation is derived by seeking solutions $h = h(y)$, $y = x - st$ of (6.1) (again, we take $D = 0$), and integrating once from $y = -\infty$:

$$-s\,(h - h_-) + f(h) - f(h_-) = -h^3\, h'''. \tag{6.2}$$

To this equation we add boundary conditions $h(\pm\infty) = h_\pm$. Of course, we have

$$s = \overline{a}(h_-, h_+) := h_- + h_+ + h_-^2 + h_-\, h_+ + h_+^2,$$

since $h_\pm$ must be equilibria for the ODE (6.2).

With $h_+ = 0.1$, it was found that for an interval $I = (h_+, h_{max})$ of values of h_-, there are (sometimes multiple) traveling waves approximating the compressive shock from h_- to h_+. Moreover, in the interior of this range, there is a value $h_- = h_-^* \in I$ for which there is additionally a traveling wave approximating an undercompressive shock from $\tilde{h}_- > h_-^*$, with $\overline{a}(h_-^*, h_+) = \overline{a}(\tilde{h}_-, h_+)$, to h_+. For $h_{max} < h_- < \tilde{h}_-$, there are no traveling waves connecting h_- to h_+.

This structure can be understood from the phase portraits of equation (6.2), as explained in [5]; our purpose in the present section is to connect the structure with the kinetic relation and the nucleation condition introduced in this paper. First of all, the undercompressive traveling wave from $\tilde{h}_-$ to h_+ represents the kinetic relation. That is, since $\tilde{h}_-$ and h_-^* depend on h_+, we can let

$$\varphi^\flat(h_+) = \tilde{h}_-, \quad \varphi^\sharp(h_+) = h_-^*. \tag{6.3}$$

Similarly, the upper limit h_{max} on h_- for the existence of compressive traveling waves can be taken to represent the nucleation condition. That is, we can set

$$\varphi^N(h_+) = h_{max}. \tag{6.4}$$

With these identifications, the simulations of initial value problems for equation (6.1) can be understood in terms of the hyperbolic theory of this paper.

However, there may be some features described in [5] in which the dissipation plays a more detailed role, which are not captured by the hyperbolic theory. For example, initial data with a narrow plateau, say with width $a > 0$ can give a single wave solution where a broader ridge leads to a double wave structure. This cannot be explained by wave interactions at the hyperbolic level, and it seems that for small a the dissipative effects dominate the hyperbolic wave structure initially. By scaling x and t in equation (6.1) by a large constant $A > 0$, a small parameter $\epsilon = A^{-3}$ is introduced as a coefficient in front of the fourth-order diffusion. It would be reasonable to expect that for $a > A^{-1} = \epsilon^{1/3}$, the hyperbolic structure would be recovered in simulations of the dissipative equation. It would be interesting to do the numerical experiments. (See also the discussion in Section 7 below.)

7. Concluding Remarks

In this paper, we have formulated a theory for a scalar conservation law, motivated by the regularized equation (6.1), containing both second order and fourth order diffusion. Other regularizations leading to nonclassical shocks have second order diffusion and dispersion, such as the modified KdV-Burgers equation [4,15,17]. However, for these regularizations, it appears that no nucleation condition is needed to explain the wave structure of solutions observed in numerical solutions of initial value problems. This can be explained in part through analysis of traveling waves: for second order diffusion plus third order dispersion, **Lax shocks lose traveling wave profiles precisely when an undercompressive shock admits a traveling wave profile.** In other words, the nucleation condition and kinetic relation coincide.

To put some perspective on the results obtained in this paper, consider the equation

$$\partial_t u + \partial_x f(u) = \alpha\, u_{xx} + \beta\, u_{xxx} - \gamma\, u_{xxxx} \tag{7.1}$$

in which all three regularizations are included.

As far as the Riemann problem is concerned, every limiting solution u obtained when $\alpha, \beta, \gamma \to 0$ (for some definite ratios α^2/β and α^3/γ) must be one of the solutions constructed in Section 3, where we described the general selection framework based on a nonclassical set $\mathcal{N}$. This is a consequence of the following two observations :

1. Any (formal) limit $u = \lim_{\alpha,\beta,\gamma\to 0} u^{\alpha\beta\gamma}$ of the equation (7.1) satisfies the entropy inequality
$$\partial_t \frac{u^2}{2} + \partial_x g(u) \le 0, \qquad g(u) := \int^u f'(u)\, u\, du, \tag{7.2}$$
as follows immediately from the identity
$$\partial_t \frac{u^2}{2} + \partial_x g(u) = -\alpha\, |u_x|^2 - \gamma\, |u_{xx}|^2 \partial_x R^{\alpha\beta\gamma}, \tag{7.3}$$
where $\partial_x R^{\alpha\beta\gamma}$ is a conservative term, vanishing with $\alpha, \beta, \gamma \to 0$.
2. For any given Riemann data, the set of all Riemann solutions satisfying a single entropy inequality can be parametrized by a single real parameter. (The complete description of all Riemann solutions is provided in [17].)

Such limiting solutions are endowed with a specific kinetic function $\varphi^\flat$ and a specific nonclassical set $\mathcal{N}$. It would be very interesting to know if the particular form of the nucleation solver (3.8) associated with a threshold function φ^N captures the various limiting solutions of (7.1) accurately, or whether the more general framework based on a nonclassical set $\mathcal{N}$ is needed. It must be pointed out that it is also quite possible that the hyperbolic theory is not the right setting to describe the limits of (7.1) (assuming that the limits even exist).

Extensive numerical computations of the kinetic function $\varphi^\flat$ have been performed by the first author and his collaborators for various examples for which the kinetic function gave a satisfactory description of the singular limits. The dependence of the kinetic function with respect to the diffusion/dispersion ratio, the form of the regularization, the order of accuracy of the scheme, etc were studied numerically. See in particular [7, 12, 18,20]. In addition, the kinetic function was used in combination with the Glimm and wave front tracking schemes [8, 16, 17] to compute solutions at the hyperbolic level of modeling.

Establishing the existence of the traveling waves for the thin film model ((7.1) with $\alpha = \beta = 0$) turned out to be challenging [6]. On the other hand, when $\gamma = 0$, the traveling wave equation is simpler and the analysis provides specific informations on the kinetic function.

An open problem is to show, for the full model (7.1), the existence of the kinetic function and to analyse its monotonicity properties and asymptotic behavior.

In addition, it would be interesting to continue the investigation numerically and to tabulate the nucleation function and investigate its properties, as it does not seem to be tractable analytically, even when $\alpha = \beta = 0$. Performing further simulations of the PDE to compare directly with predictions of the hyperbolic theory, with kinetics and nucleation given by the tabulated functions, will shed some light on the validity of the framework proposed in this paper. While the kinetic relation is undoubtedly correct, the nucleation condition is somewhat arbitrary, and it may be that a different choice of nucleation condition will give a better hyperbolic representation of the diffusive PDE solutions.

As described earlier, nucleation conditions were introduced originally for systems of mixed type associated with dynamic phase transitions [1]. For the strictly hyperbolic p-system, nucleation conditions have not been needed to specify a unique solution of the Riemann problem [19, 23]; there is a unique solution whose shock waves possess traveling wave solutions of a diffusion-dispersion regularization (generally referred to as viscosity-capillarity). In principle, if higher order regularization were called for, then a nucleation condition could be specified along the lines of the one introduced here for scalar equations, in order to reproduce, at the hyperbolic level, solutions of the regularized system. However, there is no physical context (to our knowledge) motivating the introduction of such a condition.

On the other hand, for nonstrictly hyperbolic systems with a quadratic flux (of type II [22]), there are solutions for the same Riemann data using either a traveling wave condition (which admits nonclassical waves), or using only classical waves. Here, it would be interesting to formulate a kinetic relation for nonclassical shocks, to characterize all nonclassical solutions of the Riemann problem, and to describe a nucleation or selection condition to specify a unique solution of the Riemann problem.

Acknowledgements:. MS was partially supported by National Science Foundation grant DMS-0073841. PGL was partially suported by the Centre National de la Recherche Scientifique (CNRS) and by the University of Cambridge. The authors gratefully acknowledge the support and hospitality of the Isaac Newton Institute for Mathematical Sciences, University of Cambridge, where this research was performed during the Semester Program "Nonlinear Hyperbolic Waves in Phase Dynamics and Astrophysics".

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