

## MIT Open Access Articles

### *Discrete and continuous scalar conservation laws*

The MIT Faculty has made this article openly available. **Please share** how this access benefits you. Your story matters.

**Citation:** Abeyaratne, R., and J. K. Knowles. "Discrete and Continuous Scalar Conservation Laws." *Mathematics and Mechanics of Solids* 16, no. 3 (May 1, 2011): 283–303.

**As Published:** <http://dx.doi.org/10.1177/1081286510382821>

**Publisher:** Sage Publications

**Persistent URL:** <http://hdl.handle.net/1721.1/87764>

**Version:** Author's final manuscript: final author's manuscript post peer review, without publisher's formatting or copy editing

**Terms of use:** Creative Commons Attribution-Noncommercial-Share Alike



## Discrete and Continuous Scalar Conservation Laws

Rohan Abeyaratne<sup>1</sup>

The SMART Center  
Massachusetts Institute of Technology  
3 Science Drive 2, Mail Code S16-05-08  
Singapore 117543  
rohan@smart.mit.edu

James K. Knowles

Division of Engineering and Applied Science  
California Institute of Technology  
Pasadena, CA 911 25

### Abstract

Motivated by issues arising for discrete second-order conservation laws and their continuum limits (applicable, for example, to one-dimensional nonlinear spring-mass systems), here we study the corresponding issues in the simpler setting of first-order conservation laws (applicable, for example, to the simplest theory of traffic flow). The discrete model studied here comprises of a system of first-order nonlinear differential-difference equations; its continuum limit is a one-dimensional scalar conservation law. Our focus is on issues related to discontinuities – shock waves – in the continuous theory and the corresponding regions of rapid change in the discrete model. In the discrete case, we show that a family of new conservation laws can be deduced from the basic one, while in the continuous case we show that this is true only for smooth solutions. We also examine how well the continuous model approximates rapidly changing solutions of the discrete model, and this leads us to derive an improved continuous model which is of second-order. We also consider the form and implications of the second law of thermodynamics at shock waves in the scalar case.

### 1 Introduction

Consider a one-dimensional array of mass points connected by nonlinearly elastic springs — a “chain of atoms”. When set in motion, this system responds as a conservative discrete mechanical system governed by  $N$  coupled nonlinear second-order ordinary differential equations for the positions of the  $N$  mass points as functions of time. During any motion of the chain, the rate of change of the sum of the kinetic

---

<sup>1</sup>Corresponding author. The work described in this paper, and a preliminary version of the manuscript, were completed before the passing away of Jim Knowles in November 2009. Some final changes to the manuscript were subsequently made by Rohan Abeyaratne.

energies of the masses and the stored energies in the springs coincides with the rate at which work is supplied by the external forces, so that dissipation is absent.

However if there are many closely-spaced masses, it is natural to take an appropriate limit of the discrete system and approximate it as a one-dimensional nonlinearly elastic continuum – an “elastic bar”. If the bar is set in motion, and if the motion is smooth, the response is that of a conservative continuum-mechanical system governed by a pair of first-order partial differential equations (or equivalently a single second-order nonlinear partial differential equation). During such a smooth motion, the rate of change of the sum of the kinetic and strain energies of the bar coincides with the rate at which external work is supplied, just as in the discrete system.

In the continuum-mechanical case, however, the external loading may provoke a dynamical response that involves propagating strain discontinuities, so that the resulting motion is *not* smooth. Such discontinuities, i.e. *shock waves*, are agents of dissipation if the constitutive response of the bar is nonlinear. When they occur in the continuum theory, the rate of change of total energy does *not* coincide with the rate of work supplied to the bar by external sources. This has no analog in the underlying discrete model from which the continuous model was derived. Thus the discrete and continuous versions of the energy conservation law differ when shocks are present in the latter.

To see another manifestation of this, let  $\lambda(x, t)$  and  $v(x, t)$  be the stretch and velocity respectively in the bar at time  $t$ , of the particle which was located at  $x$  in some reference configuration. For smooth motions of the bar, these fields obey the conservation laws

$$\lambda_t = v_x, \quad v_t = [W'(\lambda)]_x, \quad [v^2/2 + W(\lambda)]_t = [vW'(\lambda)]_x, \quad (1)$$

related to compatibility, momentum and energy where  $W(\lambda)$  is the elastic potential that characterizes this material; and the subscripts  $x$  and  $t$  represent partial differentiation. It may be readily shown that  $(1)_3$  follows from  $(1)_{1,2}$ . If the motion involves a shock wave located at  $x = s(t)$ , the jump conditions across the shock wave associated with the three conservation laws are

$$\dot{s}[\lambda] + [v] = 0, \quad \dot{s}[v] + [[W'(\lambda)]] = 0, \quad \dot{s}[v^2/2 + W(\lambda)] + [[vW'(\lambda)]] = 0, \quad (2)$$

respectively. However in contrast to the field equations for smooth motions above, the jump condition  $(2)_3$  does *not* follow from the jump conditions  $(2)_{1,2}$ .

The relation between discrete and continuous models of a dense chain of particles has been widely studied. Important recent contributions include those of Rosenau [8],

Purohit [7], and Dryer, Hoffman, and Mielke [3]. Further work on this subject may be found in the references cited in these papers.

In the present paper, we wish to discuss the relation between discrete and continuous conservation laws in a context that is mathematically simpler than that of the physical system mentioned above. Here the analog of the continuous model of the elastic bar is a one-dimensional *scalar* conservation law that, when accompanied by the simplest type of constitutive relation, leads to a first-order quasilinear partial differential equation for a scalar unknown function  $\rho(x, t)$ :

$$\rho_t + [Q(\rho)]_x = 0. \quad (3)$$

A partial differential equation of this kind arises, for example, in the widely used model of traffic flow proposed originally by Lighthill and Whitham [6, 10]. In this application,  $\rho(x, t)$  stand for the vehicular traffic *density*. If the density does not vary continuously but suffers a discontinuity at a location  $x = s(t)$ , the jump condition

$$-s' [[\rho]] + [[Q(\rho)]] = 0 \quad (4)$$

associated with (3) must hold at the shock.

Underlying this simpler scalar setting is also a related discrete formulation (e.g. think of vehicular traffic). The discrete model involves a set of densities  $\underline{\rho}(t) = \{\rho_0(t), \rho_1(t), \rho_2(t), \dots, \rho_N(t)\}$  which obey a system of  $N$  first-order ordinary differential equations

$$\dot{\rho}_n + \frac{1}{h} \left\{ Q(\rho_n(t)) - Q(\rho_{n-1}(t)) \right\} = 0, \quad \text{for } n = 0, 1, 2, \dots, N, \quad (5)$$

where the length  $h$  is the spacing in the reference configuration. There is no notion of a shock wave in the discrete setting. *As in the context of the chain-of-atoms discussed above, we shall view the discrete system (5) as the fundamental one, with the one-dimensional scalar partial differential equation (3) being its continuum limit.* Our starting point in this paper will be the *global balance law associated with the discrete model*, and our focus will be on regions of rapid change in the density. We present *three results* in this paper.

*The first result*, obtained in Section 5, is analogous to the issue described at the beginning of this section for the mechanical problem. Just as the conservation laws  $(1)_{1,2} \rightarrow (1)_3$  in the case of an elastic bar, we shall show that for smooth solutions,

the continuous scalar conservation law (3) implies *an entire family* of new conservation laws

$$[\mathcal{N}(\rho)]_t + [\mathcal{G}(\rho)]_x = 0 \quad (6)$$

where  $\mathcal{N}(\rho)$  is an *arbitrary* invertible smooth function and  $\mathcal{G}$  is suitably related to  $\mathcal{N}$ . Again, as for the elastic bar, for nonsmooth solutions the jump condition (4) does *not* imply the jump condition associated with (6), i.e. in general

$$-\dot{s} \llbracket \mathcal{N}(\rho) \rrbracket + \llbracket \mathcal{G}(\rho) \rrbracket \neq 0 \quad (7)$$

no matter what the choice of  $\mathcal{N}$ . On the other hand the system of discrete conservation laws (5) *always* leads to the alternative family of new conservation laws

$$[\mathcal{N}(\rho_n)]_t + \frac{1}{h} [\mathcal{G}_n(\rho(t)) - \mathcal{G}_{n-1}(\rho(t))] = 0, \quad \text{for } n = 0, 1, 2, \dots, N, \quad (8)$$

there being no analog of shock waves in the discrete setting. This is analogous to the momentum equation always implying the energy equation for a discrete chain of particles but not for a continuous system.

*The second result* involves a specific boundary-initial value problem – the so-called signaling problem – which we use as a vehicle to examine how well the continuous model approximates the discrete model in the vicinity of a shock wave. The linear case is studied first in Section 6 and the nonlinear case in Section 7. It is seen that the continuous model provides a poor approximation near a shock wave in both cases. An improved (second-order) continuous model is therefore derived from the discrete model and this leads to good agreement. In the linear case the signaling problem for all three models is solved analytically. In the nonlinear case the discrete model is solved numerically, the continuous model analytically, and the improved second-order continuous model using a boundary layer method.

*The third result* pertains to the role of the second law of thermodynamics in the case of the one-dimensional scalar conservation law. In Section 4 the entropy inequality at a shock wave is derived under certain assumptions, leading to the notion of the *driving force* on a shock wave. It is observed that this inequality is weaker than both the Lax and Oleinik selection criteria for picking shock waves. Therefore for the one-dimensional scalar conservation law, the field equation, jump condition and thermodynamic entropy inequality are expected to be *insufficient* in general for providing unique solutions to initial-boundary value problems.

## 2 Formulation

Consider a fixed interval  $[0, L]$  of the  $x$ -axis and divide it into  $N$  subintervals of equal length  $h = L/N$ . Set  $x_n = nh$ ,  $n = 0, 1, 2, \dots, N$ , so that  $x_0 = 0$  and  $x_N = L$ .

Let  $\underline{\rho}(t)$  stand for the finite sequence of *densities*  $\{\rho_0(t), \rho_1(t), \dots, \rho_N(t)\}$  and let  $\underline{q}(t)$  stand for the finite sequence of *fluxes*  $\{q_0(t), q_1(t), \dots, q_N(t)\}$ . Here we are considering the motion along the  $x$ -axis of certain discrete entities: the number of these entities located in the interval  $(x_n - h/2, x_n + h/2]$  at time  $t$  is  $h\rho_n(t)$ ; and the number of these entities crossing the location  $x_n$  per unit time at time  $t$  is  $q_n(t)$ . Suppose that  $\underline{\rho}$ ,  $\underline{q}$  satisfy the *global balance law*

$$\frac{d}{dt} \left\{ \sum_{n=i}^j h \rho_n(t) \right\} + q_j(t) - q_{i-1}(t) = 0, \quad t \geq 0, \quad (9)$$

for all integers  $i, j$  such that  $1 \leq i \leq j \leq N$ . Here we have chosen an arbitrary segment  $[x_i, x_j]$  and the first term in (9) represents the rate of increase of the number of entities in this interval whose density is  $\underline{\rho}$  and this is balanced by the flux of these entities entering the segment across its two ends  $x_j$  and  $x_{i-1}$  as represented by the next two terms. It can be readily seen that  $\underline{\rho}$ ,  $\underline{q}$  satisfy the global balance law (9) if and only if their elements satisfy the system of *local conservation laws*

$$\dot{\rho}_n(t) + \frac{q_n(t) - q_{n-1}(t)}{h} = 0, \quad n = 1, 2, \dots, N, \quad t \geq 0. \quad (10)$$

Additional information is needed in order to solve for the  $\rho$ 's and  $q$ 's. This could, for example, be a second balance law or alternatively a constitutive law. We consider the latter case here and suppose that the elements of the sequences  $\underline{\rho}$  and  $\underline{q}$  are related by a constitutive law

$$q_n = Q(\rho_n), \quad n = 0, 1, 2, \dots, N, \quad (11)$$

where the constitutive function  $Q$  is prescribed and has the following properties: we assume that  $Q$  is defined and twice continuously differentiable on  $[0, \rho_{max}]$  for some  $\rho_{max} > 0$ . Moreover, we suppose that

$$Q(0) = 0, \quad c_0 = Q'(0) > 0, \quad \text{and} \quad Q(\rho) > 0 \text{ for } 0 < \rho < \rho_{max}. \quad (12)$$

Note that  $c_0$  has the dimension of speed.

Combining (11) with (10) leads to the following set of  $N$  differential-difference equations:

$$\dot{\rho}_n + \frac{Q(\rho_n) - Q(\rho_{n-1})}{h} = 0, \quad n = 0, 1, 2, \dots, N, \quad t \geq 0. \quad (13)$$

In order to solve this system of equations for  $\underline{\rho}(t)$ , one needs to prescribe the initial conditions  $\underline{\rho}(0)$ , and a boundary condition in the form of, say, giving  $\rho_0(t)$  for all  $t \geq 0$ . *This is the basic problem that we wish to study.*

### 3 The Continuous Version.

Before we take the continuum limit of the preceding set of discrete equations we first nondimensionalize the various quantities. For this purpose we choose the speed  $c_0$  and the two lengths  $h$  and  $L$ , assuming that

$$\varepsilon = \frac{h}{L} \ll 1$$

is a small parameter. *Moreover, we suppose that we are interested in the variations of  $\underline{\rho}$  and  $\underline{q}$ , not at the “microscopic” scale  $h$ , but rather at the “macroscopic” scale  $L$ .* Thus we non-dimensionalize the various quantities as follows:

$$\bar{x}_n = x_n/L = n\varepsilon, \quad \bar{t} = t(c_0/L), \quad \bar{\rho}_n(\bar{t}) = h\rho_n(t), \quad \bar{q}_n(\bar{t}) = hq_n(t)/c_0, \quad (14)$$

and introduce the nondimensional version of the function  $Q$  by

$$\bar{Q}(\bar{\rho}) = \frac{h}{c_0} Q(\bar{\rho}/h). \quad (15)$$

Observe that

$$\bar{x}_n = \bar{x}_{n-1} + \varepsilon, \quad \dot{\bar{\rho}}_n = \frac{c_0}{\varepsilon L^2} \frac{d\bar{\rho}_n}{d\bar{t}}, \quad q_n - q_{n-1} = \frac{c_0}{\varepsilon L} [\bar{q}_n - \bar{q}_{n-1}]. \quad (16)$$

The global balance law (9) and the local conservation law (10) now take the respective nondimensional forms

$$\frac{d}{d\bar{t}} \left\{ \sum_{n=i}^j \varepsilon \bar{\rho}_n(\bar{t}) \right\} + \bar{q}_j(\bar{t}) - \bar{q}_{i-1}(\bar{t}) = 0, \quad t \geq 0, \quad (17)$$

$$\frac{d\bar{\rho}_n}{d\bar{t}} + \frac{\bar{q}_n - \bar{q}_{n-1}}{\varepsilon} = 0. \quad (18)$$

They are supplemented by the constitutive law

$$\bar{q}_n = \bar{Q}(\bar{\rho}_n), \quad n = 0, 1, 2, \dots, N. \quad (19)$$

Note from (12)<sub>2</sub> and (15) that

$$\bar{Q}(0) = 0, \quad \bar{Q}'(0) = 1. \quad (20)$$

Now we may construct the continuum limit of (17) – (19) by letting  $\varepsilon = h/L \rightarrow 0$ . Assume that the variations in the density  $\rho_n$  and flux  $q_n$  occur over distances of  $O(L)$ . Then the variations in  $\bar{\rho}_n$  and  $\bar{q}_n$  occur over distances of  $O(1)$ . Thus we assume that there are “well-behaved” functions  $\bar{\rho}(\bar{x}, \bar{t})$  and  $\bar{q}(\bar{x}, \bar{t})$  on  $0 \leq \bar{x} \leq 1, \bar{t} \geq 0$ , such that

$$\bar{\rho}_n(\bar{t}) = \bar{\rho}(\bar{x}_n, \bar{t}) = \bar{\rho}(\varepsilon n, \bar{t}), \quad \bar{q}_n(\bar{t}) = \bar{q}(\bar{x}_n, \bar{t}) = \bar{q}(\varepsilon n, \bar{t}), \quad (21)$$

and whose partial derivatives with respect to  $\bar{x}$  and  $\bar{t}$  are also  $O(1)$ .

First consider the discrete global balance law (17) which can be written as

$$\frac{d}{d\bar{t}} \left\{ \sum_{n=i}^j \bar{\rho}(\bar{x}_n, \bar{t}) [\bar{x}_n - \bar{x}_{n-1}] \right\} + \bar{q}(\bar{x}_j, \bar{t}) - \bar{q}(\bar{x}_i - \varepsilon, \bar{t}) = 0,$$

Recall that  $\bar{x}_n - \bar{x}_{n-1} = \varepsilon$ . In the limit  $\varepsilon \rightarrow 0$  this leads to the following *global balance law for the continuous case*:

$$\frac{d}{d\bar{t}} \left\{ \int_{\bar{x}_i}^{\bar{x}_j} \bar{\rho}(\bar{x}, \bar{t}) d\bar{x} \right\} + \bar{q}(\bar{x}_j, \bar{t}) - \bar{q}(\bar{x}_i, \bar{t}) = 0 \quad (22)$$

which must hold for all  $\bar{x}_i, \bar{x}_j$  in  $[0, 1], \bar{t} \geq 0$ . Next we turn to the discrete local conservation law (18). Note first that

$$\frac{d}{d\bar{t}} \bar{\rho}_n(\bar{t}) = \frac{\partial}{\partial \bar{t}} \bar{\rho}(\bar{x}_n, \bar{t}) \quad \text{and} \quad (23)$$

$$\bar{q}_{n-1}(\bar{t}) = \bar{q}(\bar{x}_{n-1}, \bar{t}) = \bar{q}(\bar{x}_n - \varepsilon, \bar{t}) = \bar{q}(\bar{x}_n, \bar{t}) - \varepsilon \frac{\partial}{\partial \bar{x}} \bar{q}(\bar{x}_n, \bar{t}) + O(\varepsilon^2). \quad (24)$$

Therefore in the limit  $\varepsilon \rightarrow 0$ , equation (18) yields the following partial differential equation representing the *local conservation law for the continuous case*:

$$\frac{\partial}{\partial \bar{t}} \bar{\rho}(\bar{x}_n, \bar{t}) + \frac{\partial}{\partial \bar{x}} \bar{q}(\bar{x}_n, \bar{t}) = 0. \quad (25)$$

The constitutive law is clearly

$$\bar{q}(\bar{x}, \bar{t}) = \bar{Q}(\bar{\rho}(\bar{x}, \bar{t})). \quad (26)$$

If  $\bar{\rho}$  and  $\bar{q}$  are continuous and piecewise continuously differentiable, a direct calculation shows that (22) holds *if and only if* the local conservation law (25) holds. This is the precise analog of the fact that in the discrete case, the sequences  $\underline{\rho}(t)$  and  $\underline{q}(t)$  satisfy the global balance law (9) *if and only if* they satisfy the local conservation law (10).



From hereon we shall drop the overbars and simply keep in mind that we are working with the nondimensional quantities. In particular we write (25) as

$$\rho_t + q_x = 0 \tag{27}$$

where the subscripts  $t$  and  $x$  indicate partial derivatives. Together with  $q = Q(\rho)$ , equation (27) gives

$$\rho_t + Q'(\rho)\rho_x = 0. \tag{28}$$

A continuous, piecewise smooth function  $\rho$  that satisfies (28) is a *strong solution*.

On the other hand it is well known that solutions of (28), even with smooth initial data, can develop discontinuities (shocks) in finite time. One is therefore led to consider solutions  $\rho$  of (28) that are continuous on  $[0, 1] \times [0, \infty)$  *except* for a jump discontinuity along, say, a curve  $x = s(t)$ , while remaining piecewise continuously differentiable elsewhere. In this case (22) holds *if and only if*

$$\rho_t + q_x = 0 \text{ for } x \neq s(t), \quad [[q]] - \dot{s}[[\rho]] = 0 \text{ for } x = s(t), \tag{29}$$

where, for example,  $[[\rho]]$  denotes  $[[\rho]] = \rho_+ - \rho_- = \rho(s(t)+, t) - \rho(s(t)-, t)$ . Such a discontinuity is a *shock wave* and  $\dot{s}$  is the shock velocity. If  $\rho$  is piecewise continuous and piecewise smooth, it constitutes a *weak solution* of (28) if it satisfies (29)<sub>1</sub> where it is continuous and the jump conditions (29)<sub>2</sub> at every discontinuity  $x = s(t)$ .

*There is no analog of a weak solution in the original discrete problem.*

It is also worth noting that the continuous model (28) was derived under the assumption that the variation of the fields  $\rho(x, t)$  and  $q(x, t)$  occur on a length scale of  $O(1)$ . This is clearly not the case at a shock wave where these fields vary discontinuously. Therefore there is no reason to expect the continuous model derived here to be a good approximation of the discrete model in the vicinity of a shock. A different scaling using a “microscopic” length such as  $h$  would be needed to derive an appropriate description of shocks from the discrete model. We do not pursue this here.

## 4 Entropy.

### 4.1 Global and local considerations in the continuum model.

In the continuum formulation of Section 3, in addition to the basic global balance law (22), the physics of the underlying problem would also require that the second law of

thermodynamics hold. Typically, one would have an entropy density  $\eta(x, t)$  and an entropy flux  $g(x, t)$  such that the rate of change of entropy associated with a segment  $[x_1, x_2]$ , say  $\Gamma(t; x_1, x_2)$ , is the rate of change of total entropy in that segment plus the flux of entropy into that segment.

$$\Gamma(t; x_1, x_2) = \frac{d}{dt} \int_{x_1}^{x_2} \eta(x, t) dx + g(x_2, t) - g(x_1, t). \quad (30)$$

Proper characterization of the entropy density and the entropy flux requires further information about the underlying physical problem. In the absence of such information, here we take the standard mathematical approach (see for example Section 7.4 of Dafermos [2]) and suppose that there are constitutive relations

$$\eta = \mathcal{N}(\rho), \quad g = \mathcal{G}(\rho) \quad (31)$$

that relate the entropy density  $\eta$  and the entropy flux  $g$  to the basic field  $\rho$ . Suppose further that

- (i) entropy is only produced at a shock wave;
- (ii) the entropy production rate at a shock wave can be written in terms of the product of a “driving force”  $f$  and the flux  $\dot{s}$  as is often the case in physical problems, (see, for example, Chapter 14 of Callen [1] or Lecture 7 of Truesdell [9]); and
- (iii) the driving force  $f$  depends solely on the states immediately on either side of the shock, i.e. that  $f = f(\rho_+, \rho_-)$  where  $\rho_{\pm} = \rho(s(t) \pm, t)$ .

Knowles [4] has shown that this is possible if the constitutive functions for the entropy density and the entropy flux are taken to be

$$\mathcal{N}(\rho) = - \int_0^{\rho} Q(r) dr, \quad \mathcal{G}(\rho) = -\frac{1}{2}Q^2(\rho). \quad (32)$$

For the remainder of *this* sub-section it is assumed that  $\mathcal{N}$  and  $\mathcal{G}$  are given by (32).

Since  $\mathcal{N}'(\rho) = -Q(\rho) < 0$  we can invert (31)<sub>1</sub> and substitute the result into (31)<sub>2</sub> to get

$$g = G(\eta) = \mathcal{G}(\mathcal{N}^{-1}(\eta)). \quad (33)$$

Suppose that  $\rho(x, t)$  is a *strong solution* of (28). Then it can be readily verified that the entropy production rate vanishes:

$$\Gamma(t; x_1, x_2) = \frac{d}{dt} \int_{x_1}^{x_2} \eta(x, t) dx + G(\eta(x_2, t)) - G(\eta(x_1, t)) = 0. \quad (34)$$

On the other hand if  $\rho$  is a *weak solution* of (28) that is continuous on  $[0, 1]$  except at  $x = s(t)$  where it jumps. Then a straightforward calculation shows that the entropy production rate does not vanish in general and that it is given by

$$\Gamma(t; x_1, x_2) = \frac{d}{dt} \int_{x_1}^{x_2} \eta(x, t) dx + G(\eta(x_2, t)) - G(\eta(x_1, t)) = \llbracket G(\eta) \rrbracket - \dot{s} \llbracket \eta \rrbracket \neq 0; \quad (35)$$

thus  $\llbracket G(\eta) \rrbracket - \dot{s} \llbracket \eta \rrbracket$  represents the *entropy production rate associated with the shock*. As shown by Knowles [4], after some algebra this can be written as

$$\Gamma(t; x_1, x_2) = f \dot{s} \quad (36)$$

where the driving force  $f$  at the shock is given by

$$f(\rho_+, \rho_-) = \int_{\rho_-}^{\rho_+} Q(\rho) d\rho - \frac{Q(\rho_+) + Q(\rho_-)}{2} \llbracket \rho \rrbracket. \quad (37)$$

The second law of thermodynamics requires that  $\Gamma(t; x_1, x_2) \geq 0$  in all processes and for all segments  $[x_1, x_2]$  whence we must have

$$f(\rho_+(t), \rho_-(t)) \dot{s}(t) \geq 0 \quad (38)$$

at every shock. *Thus in addition to the jump condition (29)<sub>2</sub>, the entropy inequality (38) is to be imposed at all shocks.*

## 4.2 Global and local considerations in the discrete model.

Analogous to the continuous case, let us introduce the entropy density  $\underline{\eta} = \{\eta_0(t), \eta_1(t), \dots, \eta_N(t)\}$  and the entropy flux  $\underline{g} = \{g_0(t), g_1(t), \dots, g_N(t)\}$  by

$$\eta_n = \mathcal{N}(\rho_n), \quad g_n = \mathcal{G}_n(\underline{\rho}), \quad n = 0, 1, \dots, N. \quad (39)$$

Here  $\mathcal{N}$  is given by (32)<sub>1</sub> and the corresponding entropy flux functions  $\mathcal{G}_n(\underline{\rho})$  and  $G_n(\underline{\eta})$  are taken to be defined by

$$\mathcal{G}_n(\underline{\rho}) = - \left\{ \sum_{k=1}^n [Q(\rho_k) - Q(\rho_{k-1})] Q(\rho_k) \right\}, \quad (40)$$

$$g_n = G_n(\underline{\eta}) = \mathcal{G}_n(\mathcal{N}^{-1}(\eta_1), \mathcal{N}^{-1}(\eta_2), \dots, \mathcal{N}^{-1}(\eta_N)), \quad (41)$$

for  $n = 1, 2, \dots, N$ .

If  $\underline{\rho}$  satisfies the global balance law (9) or equivalently the local conservation law (10), then a direct calculation shows that

$$\frac{d}{dt} \left\{ \sum_{n=i}^j \varepsilon \eta_n(t) \right\} + G_j(\underline{\eta}(t)) - G_{i-1}(\underline{\eta}(t)) = 0 \quad (42)$$

for  $i = 1, 2, \dots, N$ ,  $j = 1, 2, \dots, N$ ,  $i \leq j$ . Thus the entropy production rate always vanishes in the discrete case.

We have therefore shown that if  $\underline{\rho}$  satisfies the global balance law (9), (11), then  $\underline{\eta}$  necessarily satisfies the global balance law (42) for entropy. *Thus in contrast to the situation for weak solutions in the continuous case, there is no imbalance in the global balance law for entropy. The imbalance in the continuous case arises strictly because of propagating shocks.*

### 4.3 Remark: Uniqueness of solutions.

By loosening the smoothness requirements so as to admit weak solutions as well as strong solutions to the partial differential equation (28), we have increased the likelihood that an associated boundary-initial value problems might suffer from a lack of uniqueness of solutions. When (28) is not linear, it is known that a *selection criterion* is required at shock waves in order to avoid a breakdown in uniqueness of weak solutions. The two most common selection criteria are

$$\begin{aligned} Q'(\rho_-) \geq \dot{s} \geq Q'(\rho_+) & \quad \text{Lax condition} \\ \frac{Q(\rho) - Q(\rho_-)}{\rho - \rho_-} \geq \dot{s} \geq \frac{Q(\rho) - Q(\rho_+)}{\rho - \rho_+} & \quad \text{Oleinik condition} \end{aligned} \quad (43)$$

where the latter must hold for all  $\rho$  between  $\rho_-$  and  $\rho_+$ ; see for example Dafermos [2] or LeFloch [5]. If the constitutive function  $Q(\rho)$  happens to be either purely convex or purely concave, these two selection criteria both lead to

$$\left. \begin{aligned} \rho_- > \rho_+ \text{ for } Q(\rho) \text{ convex,} \\ \rho_- < \rho_+ \text{ for } Q(\rho) \text{ concave.} \end{aligned} \right\} \quad (44)$$

It is natural to wonder whether the entropy inequality  $f\dot{s} \geq 0$  leads to uniqueness of solution where  $f$  is the driving force defined previously in (37). If the constitutive function  $Q(\rho)$  happens to be either purely convex or purely concave, it can be readily

shown that the inequality  $f\dot{s} > 0$  is equivalent to the inequalities

$$\left. \begin{aligned} Q(\rho_+) &< Q(\rho_-) \text{ for } Q(\rho) \text{ convex,} \\ Q(\rho_+) &> Q(\rho_-) \text{ for } Q(\rho) \text{ concave,} \end{aligned} \right\} \quad (45)$$

which must hold at every shock. We note that the entropy inequality (45) is *weaker* than the selection criteria (44) above, and in fact, by itself, does not guarantee uniqueness of solution for boundary initial value problems.

## 5 Alternate Conservation Laws.

The results of the preceding section suggest an interesting generalization which we explore here. In the continuous case we show that a family of nontrivial transformations of the density-flux pair  $(\rho, q)$  leads to an associated *family of new conservation laws* when  $\rho, q$  is a strong solution of (22) but not when they are a weak solution. In the discrete case, the analogous transformation leads to a family of new conservation laws for all solutions.

### 5.1 Continuous case:

Consider the following transformation of the density-flux pair from  $(\rho, q) \rightarrow (\eta, g)$ :

$$\eta = \mathcal{N}(\rho), \quad g = \mathcal{G}(\rho); \quad (46)$$

here  $\mathcal{N} \in C^1([0, \infty))$  is invertible *but otherwise arbitrary*; corresponding to each  $\mathcal{N}$ , the function  $\mathcal{G}$  is defined by

$$\mathcal{G}(\rho) = \int_0^\rho \mathcal{N}'(r)Q'(r) dr. \quad (47)$$

The functions  $\mathcal{N}$  and  $\mathcal{G}$  here *need not be related* to the functions denoted by these same symbols in the preceding section. Thus, though we use the same symbols  $\eta(x, t)$  and  $g(x, t)$  here as in the preceding section, they are simply the fields defined by (46) and need not have any connection to entropy density and entropy flux.

Suppose that  $\rho(x, t), q(x, t)$  is a *strong solution* of (22). Then it can be readily verified that  $\eta(x, t), g(x, t)$  is also a strong solution of the same global balance law

$$\frac{d}{dt} \int_{x_1}^{x_2} \eta(x, t) dx + g(x_2, t) - g(x_1, t) = 0, \quad (48)$$

and the same local conservation law

$$\eta_t + g_x = 0. \quad (49)$$

The density  $\eta$  and the flux  $g$  are related by the constitutive law

$$g = G(\eta) = \mathcal{G}(\mathcal{N}^{-1}(\eta)). \quad (50)$$

Note that the preceding remark holds true *for every choice of the smooth invertible function  $\mathcal{N}$*  and therefore we have a family of new conservation laws.

It is illuminating to write the conservation laws (28) and (49) in the forms

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}Q(\rho) = 0 \quad \text{and} \quad \frac{\partial}{\partial t}\mathcal{N}(\rho) + \frac{\partial}{\partial x}\mathcal{G}(\rho) = 0 \quad (51)$$

which makes clear how the former conservation law leads to the latter for each choice of  $\mathcal{N}(\rho)$ .

On the other hand suppose that  $\rho, q$  is a *weak solution* of (22) that is continuous on  $[0, 1]$  except at  $x = s(t)$ , where it jumps. Define  $\eta$  and  $g$  by (46) and (47) for any  $\mathcal{N}$ . Then a straightforward calculation shows that in general

$$[[g]] - \dot{s} [[\eta]] \neq 0, \quad (52)$$

so that  $\eta, g$  do not satisfy the jump condition associated with (49). In fact one can show that

$$\frac{d}{dt} \int_{x_1}^{x_2} \eta(x, t) dx + g(x_2, t) - g(x_1, t) = [[g]] - \dot{s} [[\eta]], \quad (53)$$

where  $[[g]] - \dot{s} [[\eta]]$  need not vanish. This imbalance is due to the shock.

Thus if the pair  $\rho, q$  provides a strong solution of (22), then so does the pair  $\eta, g$ . However if the pair  $\rho, q$  provides a weak solution of (22), the pair  $\eta, g$  does not in general provide a weak solution (for any choice of  $\mathcal{N}$  in (46), (47)). It is easily verified that the imbalance vanishes in the special cases where either  $\mathcal{N}$  is the identity or  $Q(\rho) = \rho$ . In general however it does not vanish.

*In summary, for the continuous conservation law studied here whose associated partial differential equation is quasilinear, a nontrivial transformation  $(\rho, q) \rightarrow (\eta, g)$  preserves strong solutions of the conservation law but fails in general to preserve weak solutions.*

## 5.2 Discrete case:

As in the continuous case let us change the density, flux pair from  $(\underline{\rho}, \underline{q}) \rightarrow (\underline{\eta}, \underline{g})$  by the following transformation:

$$\eta_n = \mathcal{N}(\rho_n), \quad g_n = \mathcal{G}_n(\underline{\rho}), \quad n = 0, 1, \dots, \mathcal{N}, \quad (54)$$

where  $\underline{\eta} = \{\eta_0(t), \eta_1(t), \dots, \eta_N(t)\}$  and  $\underline{g} = \{g_0(t), g_1(t), \dots, g_N(t)\}$ . Here  $\mathcal{N} \in C^1([0, \infty))$  is invertible but *otherwise arbitrary*; and corresponding to each  $\mathcal{N}$ , the function  $\mathcal{G}_n$  is defined by<sup>2</sup>

$$\mathcal{G}_n(\underline{\rho}) = \sum_{k=1}^n [Q(\rho_k) - Q(\rho_{k-1})] \mathcal{N}'(\rho_k). \quad (55)$$

If  $\underline{\rho}, \underline{g}$  satisfies the global balance law (9) or equivalently the local conservation law (10), then a direct calculation shows that

$$\dot{\eta}_n + \frac{g_n - g_{n-1}}{\varepsilon} = 0, \quad (56)$$

and that

$$\frac{d}{dt} \left\{ \varepsilon \sum_{n=1}^j \eta_n(t) \right\} + g_j(t) - g_{i-1}(t) = 0 \quad (57)$$

for  $i = 1, 2, \dots, N$ ,  $j = 1, 2, \dots, N$ ,  $i \leq j$ .

We have therefore shown that if the pair  $\underline{\rho}, \underline{g}$  satisfies the global balance law (9), or equivalently the local conservation law (10), then so does the transformed pair  $\underline{\eta}, \underline{g}$ .

*Thus in contrast to the situation for transformed weak solutions in the continuous case, transformation does not give rise to an imbalance in the global balance law in the discrete case, no matter what the choice of  $\mathcal{N}$ .*

## 6 The Linear Signaling Problem.

The so-called signaling problem provides a convenient vehicle for studying shock waves in a simple context. Although our main interest lies in the nonlinear signaling problem, we begin here with the linear case in both the discrete and continuous settings. Thus (see (20)) we take

$$Q(\rho) = \rho.$$

---

<sup>2</sup>In the continuous case, the constitutive law  $q = Q(\rho)$  is said to be *homogeneous*; in its non-homogeneous generalization  $Q$  will depend explicitly on position  $x$ :  $Q = Q(\rho, x)$ . In the discrete case, the nonhomogeneous version of  $q_n = Q(\rho_n)$  would have  $Q$  depending explicitly on  $n$ , so that  $q_n = Q_n(\rho_n)$ . Note that while the original variables here,  $\underline{\rho}$  and  $\underline{g}$  are related by the homogeneous constitutive law (11), the transformed variables  $\underline{\eta}$  and  $\underline{g}$  are related by the *nonhomogeneous* constitutive law  $g_n = \mathcal{G}_n(\mathcal{N}^{-1}(\eta_1), \mathcal{N}^{-1}(\eta_2), \dots, \mathcal{N}^{-1}(\eta_N))$ .

### 6.1 The linear signaling problem: discrete model.

The signaling problem for the discrete system requires the determination of  $\rho_n(t)$ ,  $n = 1, 2, 3, \dots$ , satisfying the differential-difference equations (see (18), (19))

$$\dot{\rho}_n + \frac{1}{\varepsilon}(\rho_n - \rho_{n-1}) = 0 \quad \text{for } n = 1, 2, 3, \dots, t > 0; \quad (58)$$

the boundary condition

$$\rho_0(t) = r_0 = \text{constant} \quad \text{for } t > 0; \quad (59)$$

and the initial conditions

$$\rho_n(0) = 0 \quad \text{for } n = 1, 2, 3, \dots \quad (60)$$

To solve the discrete signaling problem (58) - (60) we use the Laplace transform

$$\tilde{\rho}_n(p) = \int_0^\infty e^{-pt} \rho_n(t) dt. \quad (61)$$

Transforming the differential-difference equations (58) and using the initial conditions (60) leads to the difference equation

$$\left(p + \frac{1}{\varepsilon}\right) \tilde{\rho}_n - \frac{1}{\varepsilon} \tilde{\rho}_{n-1} = 0 \quad \text{for } n = 1, 2, 3, \dots \quad (62)$$

for the transform  $\tilde{\rho}(p)$ . The general solution of (62) has the form  $\tilde{\rho}_n = A \alpha^n$ , where  $A$  and  $\alpha$  are constants to be determined. Substituting this into (62) provides  $\alpha$  whence

$$\tilde{\rho}_n(p) = A \left(\frac{1/\varepsilon}{p + 1/\varepsilon}\right)^n \quad \text{for } n = 1, 2, 3, \dots \quad (63)$$

Transforming the boundary conditions (59) gives  $\tilde{\rho}_0(p) = r_0/p$ ; this, together with the difference equation (62) with  $n = 1$  yields  $\tilde{\rho}_1(p) = r_0 p^{-1} (1/\varepsilon)(p + 1/\varepsilon)^{-1}$ . On the otherhand (63) gives  $\tilde{\rho}_1(p) = A(1/\varepsilon)(p + 1/\varepsilon)^{-1}$ . Equating these two expressions for  $\tilde{\rho}_1(p)$  gives  $A = r_0 p^{-1}$ , so that the transform of the solution to the discrete signaling problem is

$$\tilde{\rho}_n(p) = \frac{r_0}{p} \frac{(1/\varepsilon)^n}{(p + 1/\varepsilon)^n} \quad \text{for } n = 1, 2, 3, \dots \quad (64)$$

Inverting this transform gives

$$\rho_n(t) = r_0 \left(\frac{1}{\varepsilon}\right)^n \int_0^t \frac{\tau^{n-1}}{(n-1)!} \exp(-\tau/\varepsilon) d\tau, \quad (65)$$



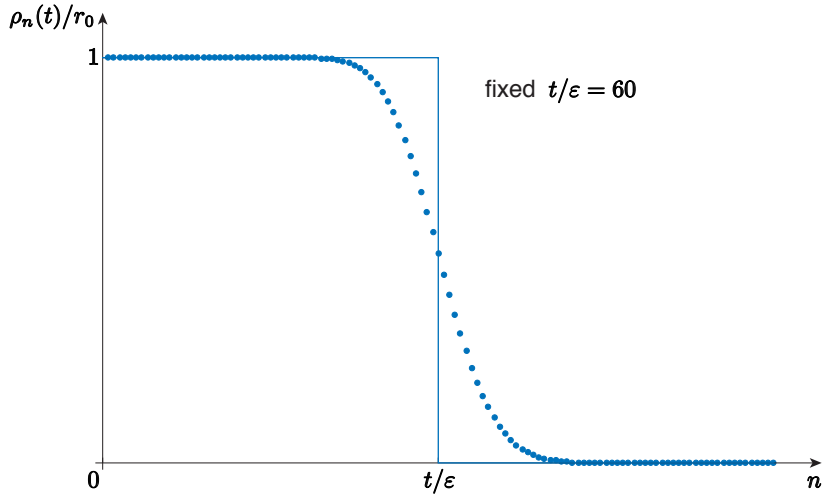


Figure 1: *The discrete linear signaling problem*: The density  $\rho_n(t)/r_0$ , as given by (68), versus position  $n$  at a fixed time  $t/\varepsilon$ . The figure is drawn at the time  $t/\varepsilon = 60$ .

which after a rescaling becomes

$$\rho_n(t) = \frac{r_0}{(n-1)!} \int_0^{t/\varepsilon} \sigma^{n-1} \exp(-\sigma) d\sigma . \quad (66)$$

The incomplete gamma function  $\Gamma(n, \tau)$  is defined by

$$\Gamma(n, \tau) = \int_\tau^\infty \sigma^{n-1} \exp(-\sigma) d\sigma \quad \text{for } n > 0, z > 0 ; \quad (67)$$

clearly,  $\Gamma(n, 0) = \Gamma(n)$  where  $\Gamma(n)$  is the standard Gamma function, which coincides with  $(n-1)!$  when  $n$  is a positive integer. We can thus write the *solution*, (66), of the *discrete signaling problem* as

$$\rho_n(t) = r_0 \left\{ 1 - \frac{\Gamma(n, t/\varepsilon)}{\Gamma(n)} \right\} \quad \text{for } n = 1, 2, 3, \dots , \quad t > 0. \quad (68)$$

Numerical values of the incomplete Gamma function, available in *Mathematica*, can be used in (68) to plot  $\rho_n(t)$  vs.  $n$  at fixed  $t$ , as depicted by the points in Figure 1.

To study the large-time behavior of  $\rho_n(t)$ , we begin by introducing

$$\chi(n, \tau) = \Gamma(n, \tau)/\Gamma(n) \quad \text{for } n = 1, 2, 3, \dots ; \quad (69)$$

integration by parts in (67) then shows that

$$\chi(n, \tau) - \chi(n-1, \tau) = \frac{\tau^{n-1}}{(n-1)!} \exp(-\tau) \quad \text{for } n = 1, 2, 3, \dots . \quad (70)$$

Summing both sides of (70) from  $n = 2$  to  $n = N(> 2)$  leads to

$$\chi(N, \tau) = \chi(1, \tau) + \exp(-\tau) \sum_{n=2}^N \frac{\tau^{n-1}}{(n-1)!} , \quad (71)$$

and, since  $\chi(1, \tau) = \exp(-\tau)$ ,

$$\chi(N, \tau) = \left\{ \sum_{n=0}^{N-1} \frac{\tau^n}{n!} \right\} \exp(-\tau) \quad \text{for } N = 1, 2, 3, \dots . \quad (72)$$

As  $\tau \rightarrow \infty$ , this immediately yields

$$\chi(N, \tau) \sim \frac{\tau^{N-1}}{(N-1)!} \exp(-\tau) \quad \text{as } \tau \rightarrow \infty . \quad (73)$$

From (68), (69), and (73), we therefore get

$$\rho_n(t) \sim r_0 \left\{ 1 - \frac{(t/\varepsilon)^{n-1}}{(n-1)!} \exp(-t/\varepsilon) \right\} \quad \text{as } t \rightarrow \infty, \text{ } n \text{ fixed} , \quad (74)$$

showing that for each  $n$ ,  $\rho_n(t) \rightarrow r_0$  exponentially fast as  $t \rightarrow \infty$ .

## 6.2 The linear signaling problem: continuous model.

In the continuous case the signaling problem requires that we find  $\rho(x, t)$  such that

$$\rho_t + \rho_x = 0 \quad \text{for } x > 0, \text{ } t > 0 , \quad (75)$$

$$\rho(0, t) = r_0 \quad \text{for } t > 0 , \quad (76)$$

$$\rho(x, 0) = 0 \quad \text{for } x > 0 . \quad (77)$$

where we have used (28) with  $Q(\rho) = \rho$ . The general solution of (75) is  $\rho = R(t - x)$  with  $R$  “arbitrary”. By (77),  $R(-x) = 0$  for  $x > 0$ , and by (76),  $R(t) = r_0$  for  $t > 0$ . It follows that  $R(z) = r_0 H(z)$  for all  $z$  where  $H(z)$  is the unit step function, and hence that the *solution of the continuous signaling problem* is

$$\rho(x, t) = r_0 H(t - x) . \quad (78)$$

This is a weak solution of (75) whose shock travels with (nondimensional) speed one.

Figure 1 includes a plot of the step-function (78). The agreement with the solution of the discrete problem in the vicinity of the shock front is seen to be poor. As noted previously, the continuous model (75) was derived from the discrete model (58) under the assumption that the variation of the field  $\rho(x, t)$  occurs on a length scale of  $O(1)$  which is clearly not the case at a shock wave where this field varies discontinuously. Therefore the lack of agreement near the shock in Figure 1 is entirely expected.

### 6.3 The linear signaling problem: second-order case.

We now obtain an improved continuous approximation to the basic discrete problem characterized by (18), (19). We start by returning to (24) and carrying out an expansion correct to<sup>3</sup>  $O(\varepsilon^3)$ :

$$q_{n-1}(t) = q_n(t) - \varepsilon q_x(x_n, t) + \frac{1}{2}\varepsilon^2 q_{xx}(x_n, t) + O(\varepsilon^3). \quad (79)$$

Thus the partial differential equation (25) is now replaced by

$$\rho_t + q_x - \frac{1}{2}\varepsilon q_{xx} = 0. \quad (80)$$

On using the constitutive law  $q = Q(\rho)$  this leads to the following second-order partial differential equation for  $\rho$ :

$$\rho_t + Q'(\rho) \rho_x - \frac{1}{2}\varepsilon\{Q'(\rho) \rho_{xx} + Q''(\rho)\rho_x^2\} = 0. \quad (81)$$

We seek solutions of this equation<sup>4</sup> that are continuous with continuous first derivatives and piecewise continuous second derivatives.

In the linear case  $Q(\rho) = \rho$  this reduces to

$$\rho_t + \rho_x - \frac{\varepsilon}{2} \rho_{xx} = 0, \quad (82)$$

and in the signaling problem we seek a solution of (82) that satisfies the boundary and initial conditions

$$\rho(0, t) = r_0 \text{ for } t > 0, \quad \rho(x, 0) = 0 \text{ for } x > 0; \quad (83)$$

in addition, it is assumed that  $\rho$  is bounded on  $[0, \infty) \times [0, \infty]$ , a requirement that serves as a second boundary condition. Let  $\mathcal{R}$  be the closed first quadrant of the  $x, t$ -plane with the origin deleted. We seek the solution  $\rho$  of the boundary-initial value problem (82), (83) in the class  $\mathcal{C}_p^2$  of functions that are continuously differentiable on  $\mathcal{R}$  with piecewise continuous second derivatives there.

Let

$$\tilde{\rho}(x, p) = \int_0^\infty e^{-pt} \rho(x, t) dt \quad (84)$$

---

<sup>3</sup>It may be noted that a similar higher order expansion in the equations for the spring-mass system leads to a partial differential equation with unstable solutions. The alternative expansion proposed by Rosenau [8] was developed to avoid this.

<sup>4</sup>Observe that one could formally obtain (81) from the original conservation law  $\rho_t + q_x = 0$  if one uses the modified constitutive law  $q = Q(\rho) - \varepsilon Q'(\rho) \rho_x/2$ .

be the Laplace transform of  $\rho(x, t)$ ; to begin with,  $p$  is taken to be real and positive. Transforming the differential equation (82) in the usual way and making use of the initial condition (83)<sub>2</sub> shows that  $\tilde{\rho}(x, p)$  must satisfy

$$\frac{\varepsilon}{2} \tilde{\rho}_{xx} - \tilde{\rho}_x - p \tilde{\rho} = 0 , \quad (85)$$

along with the transformed boundary condition

$$\tilde{\rho}(0, p) = r_0/p . \quad (86)$$

For each  $p$ ,  $\tilde{\rho}(x, p)$  must be bounded for  $0 \leq x < \infty$ ; the solution of (85) with this property that also satisfies the boundary condition (86) is

$$\tilde{\rho}(x, p) = \frac{r_0}{p} \exp \left\{ \left( 1 - (1 + 2\varepsilon p)^{1/2} \right) x/\varepsilon \right\} . \quad (87)$$

To use (87) to extend the definition of  $\tilde{\rho}(x, p)$  to the complex  $p$ -plane, we agree to take  $(1 + 2\varepsilon p)^{1/2}$  to be the function that is positive when  $p$  is real and positive and analytic in the  $p$ -plane cut from  $-\infty$  to  $-1/(2\varepsilon)$  along the negative real axis. We may then use the inversion formula for the Laplace transform to represent  $\rho(x, t)$  as an integral along a vertical path in the right half of the  $p$ -plane:

$$\rho(x, t) = \frac{r_0}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{\exp(pt)}{p} \exp \left\{ \left( 1 - (1 + 2\varepsilon p)^{1/2} \right) x/\varepsilon \right\} dp , \quad (88)$$

where  $a$  is real and positive but otherwise arbitrary.

Considered as a function of the complex variable  $p$ , the integrand in (88) has a simple pole at  $p = 0$  and a branch point of square-root type at  $p = -c/(2\varepsilon)$ . If the residue at the pole at the origin is accounted for, the contour parallel to the imaginary axis involved in the integral in (88) can be deformed to one that lies along each side of the cut to produce the following representation for the *solution*  $\rho(x, t)$  of the *linear second-order signaling problem*:

$$\begin{aligned} \rho(x, t) = & r_0 - (r_0/2) \operatorname{erfc} \left( \sqrt{2x/\varepsilon} \omega(x, t) \right) + \\ & (r_0/2) \exp(2x/\varepsilon) \operatorname{erfc} \left( \sqrt{(2x/\varepsilon)(1 + \omega^2(x, t))} \right) , \end{aligned} \quad (89)$$

where

$$\omega(x, t) = \frac{1}{2} \left( \sqrt{t/x} - \sqrt{x/t} \right) , \quad (90)$$

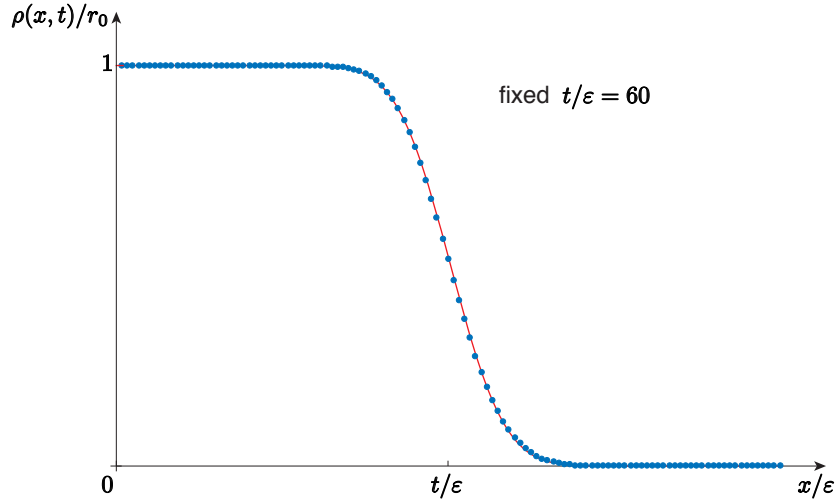


Figure 2: *The second-order continuous linear signaling problem*: The curve corresponds to a graph of the density  $\rho(x, t)/r_0$ , according to (89), versus position  $x/\varepsilon$  at a fixed time  $t/\varepsilon$ . The curve is drawn at the time  $t/\varepsilon = 60$ . The dots correspond to the solution of the discrete linear problem as was displayed in Figure 1. The excellent agreement suggests that the second-order continuous model provides a good approximation to the discrete linear model.

and  $\operatorname{erfc}(z)$  is the complementary error function:

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-\zeta^2} d\zeta . \quad (91)$$

By using simple properties of the complementary error function, one can verify that the boundary and initial conditions hold; and moreover that  $\rho(x, t) \rightarrow r_0$  as  $t \rightarrow \infty$  with  $x$  fixed, while  $\rho(x, t) \rightarrow 0$  as  $x \rightarrow \infty$  with  $t$  fixed. Figure 2 shows a plot of the density  $\rho(x, t)$  versus position  $x$  at a fixed time  $t$  based on (89). The dots correspond to the solution (68) of the discrete problem. The agreement is seen to be very good.

#### 6.4 Reconsideration of the linear second-order signaling problem: direct wave front approximation.

In preparation for considering the *nonlinear* signaling problem, we now reconsider the second-order continuous linear signaling problem and seek an alternative method, one which does not rely on linearity as does the Laplace transform procedure used above, for deriving its solution (89), or at least an approximation of the solution near the wave front  $x = t$ . If there is such a method, perhaps it could be used in the nonlinear signaling problem as well.

Let

$$\xi = x - t \tag{92}$$

and seek a solution of (82) in the form of a modulated wave traveling with unit speed:

$$\rho = \rho(\xi, t) . \tag{93}$$

We are using the same symbol  $\rho$  even though the independent variables are now  $\xi, t$ . Substituting (93) into (82) leads to the heat equation

$$\rho_t - \frac{\varepsilon}{2} \rho_{\xi\xi} = 0 , \tag{94}$$

which we now require to hold for  $-\infty < \xi < \infty, t > 0$ . Observe that we have abandoned the boundary condition  $\rho = r_0$  at  $x = 0$  and so the present process will provide (at best) an approximate solution to the exact second-order signaling problem.

As initial conditions at  $t = 0$  suppose that one has the step-function wave form

$$\rho(\xi, 0) = r_0 H(-\xi) , \tag{95}$$

where  $H$  is the Heaviside function; note that this is consistent with the initial conditions of the exact problem. The solution of the initial value problem (94), (95), is found by assuming it has the similarity form

$$\rho(\xi, t) = f\left(\xi/\sqrt{t}\right) \tag{96}$$

for some function  $f$ . Substituting (96) into (94) determines  $f$ , leading ultimately to

$$\rho(\xi, t) = A + B \operatorname{erfc}\left(-\xi/\sqrt{2\varepsilon t}\right) \tag{97}$$

where  $A, B$  are arbitrary constants. Taking the limit as  $t \rightarrow 0+$  in (97) gives

$$\lim_{t \rightarrow 0+} \rho(\xi, t) = \begin{cases} A & \text{if } \xi < 0 , \\ A + 2B & \text{if } \xi > 0 . \end{cases} \tag{98}$$

Comparing (98) and (95) gives  $A = r_0, B = -r_0/2$ , which leads through (97) to

$$\rho(\xi, t) = r_0 - \frac{r_0}{2} \operatorname{erfc}\left(-\xi/\sqrt{2\varepsilon t}\right) ; \tag{99}$$

or returning to the physical variables, to the approximation

$$\rho \sim \rho_{\text{approx}}(x, t) = r_0 \left\{ 1 - (1/2) \operatorname{erfc}\left(-\frac{x-t}{\sqrt{2\varepsilon t}}\right) \right\} . \tag{100}$$

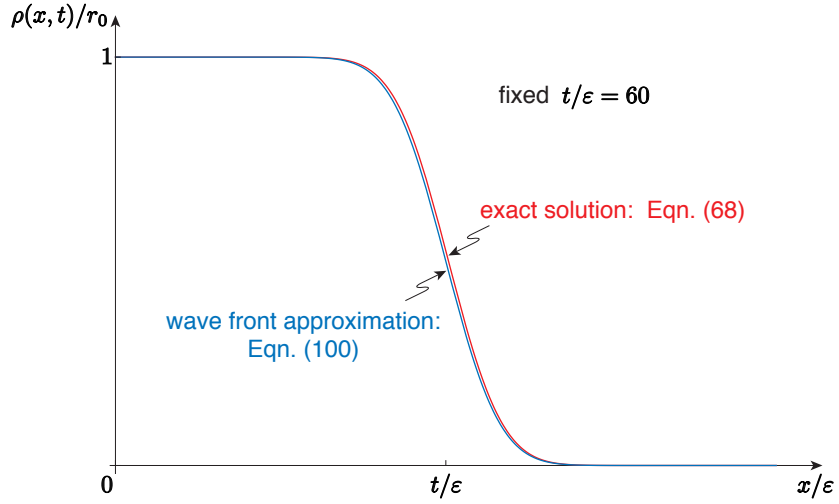


Figure 3: *Direct wave-front approximation of the second-order continuous linear signaling problem.* The density  $\rho_{\text{approx}}(x, t)/r_0$ , according to (100), versus position  $x/\varepsilon$  at a fixed time  $t/\varepsilon$ . The figure is drawn at the time  $t/\varepsilon = 60$ . The curve from Figure 2 is also shown here though it is virtually impossible to distinguish one curve from the other.

Figure 3 shows a plot of  $\rho_{\text{approx}}(x, t)$  vs.  $x$  for fixed  $t$ . It is virtually impossible to distinguish the fixed- $t$  plots of  $\rho(x, t)$  and  $\rho_{\text{approx}}(x, t)$ .

**Remark:** If we approximate the exact solution (89) near the wave front  $x = t$ , the term involving the second complementary error function in (89) is less important than the remaining two terms in (89), provided  $x$  is bounded away from 0. In fact, if  $x \geq \delta > 0$ , the second error-function term can be shown to be less than  $\sqrt{2/\pi} (\varepsilon/\delta)^{1/2}$  for all  $t$  and all  $x \geq \delta$ , which is small as  $\varepsilon \rightarrow 0$ ; the remaining terms need not be small as  $\varepsilon \rightarrow 0$ . Discarding the second error function term and approximating the remaining error function for  $x$  near  $t$  leads precisely to the approximation  $\rho \sim \rho_{\text{approx}}$  with  $\rho_{\text{approx}}$  given by (100).

## 7 The Nonlinear Signaling Problem.

### 7.1 The nonlinear signaling problem: discrete model.

The discrete signaling problem requires the determination of the infinite sequence  $\rho_1(t), \rho_2(t), \dots, \rho_n(t), \dots$  satisfying

$$\dot{\rho}_n(t) + \frac{1}{\varepsilon} \{Q(\rho_n(t)) - Q(\rho_{n-1}(t))\} = 0, \quad n = 1, 2, \dots, t > 0; \quad (101)$$

with the boundary condition

$$\rho_0(t) = r_0 = \text{constant} \quad \text{for } t > 0 ; \quad (102)$$

and the initial condition

$$\rho_n(0) = 0 \quad \text{for } n = 1, 2, \dots . \quad (103)$$

To solve this problem numerically, we begin by approximating  $\dot{\rho}_n$  by the difference quotient

$$\frac{\rho_n(t + \delta) - \rho_n(t)}{\delta} \quad (104)$$

corresponding to a given time-step  $\delta$ . We thus replace (101) by

$$\rho_n(t + \delta) = \rho_n(t) - \frac{\delta}{\varepsilon} \{Q(\rho_n(t)) - Q(\rho_{n-1}(t))\}, \quad n = 1, 2, \dots, t > 0 . \quad (105)$$

We enforce (105) only at the discrete set of times  $t = k\delta$ ,  $k = 1, 2, \dots$ , so that we seek  $w(n, k) = \rho_n(k\delta)$ , which satisfies the partial difference equation

$$w(n, k + 1) = w(n, k) - \frac{\delta}{\varepsilon} \{Q(w(n, k)) - Q(w(n - 1, k))\} \quad (106)$$

for  $n = 1, 2, \dots$ ,  $k = 1, 2, \dots$

We now specialize to *an example* for which

$$Q(\rho) = \rho + a\rho^2, \quad a > 0 , \quad (107)$$

where  $a$  is a given positive constant. We set

$$u(n, k) = \rho_n(k\delta)/r_0 = w(n, k)/r_0 , \quad (108)$$

which, with (107), reduces (106) to

$$\begin{aligned} u(n, k + 1) &= (1 - \alpha) u(n, k) + \alpha u(n - 1, k) \\ &\quad - \alpha\beta \{u^2(n, k) - u^2(n - 1, k)\} \end{aligned} \quad (109)$$

for  $n = 1, 2, \dots$ ,  $k = 1, 2, \dots$ . Here

$$\alpha = \delta/\varepsilon, \quad \beta = ar_0 . \quad (110)$$

Accompanying (109) are the side conditions

$$u(0, k) = 1, \quad k = 1, 2, \dots; \quad u(n, 0) = 0, \quad n = 0, 1, 2, \dots . \quad (111)$$

The discrete signaling problem consists of the two-dimensional difference equation (109) and the side conditions (111). Since the difference equation (109) determines  $u(n, k)$  in terms of  $u(n, k - 1)$  and  $u(n - 1, k - 1)$ , the problem is readily solved recursively with the help of *Mathematica*. Figure 4 shows the result of such a calculation.



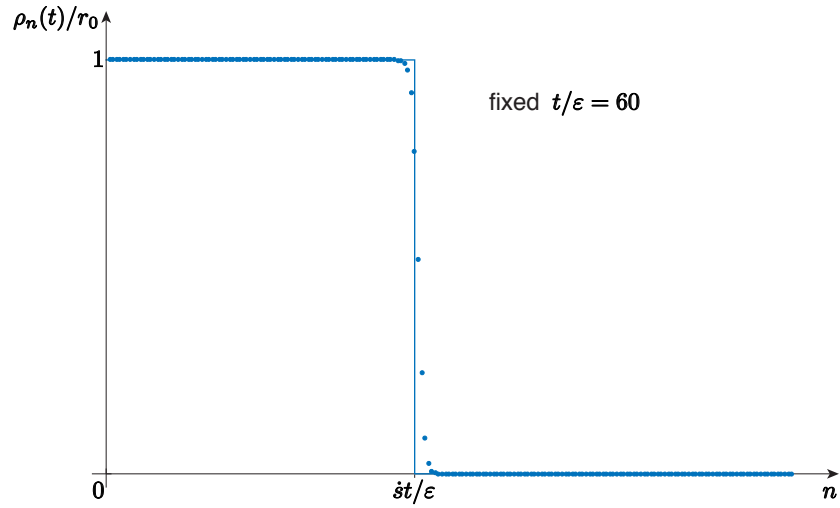


Figure 4: *The discrete nonlinear signaling problem:* The dotted curve depicts the density  $\rho_n(t)/r_0$  (found by solving (109), (111), (108) recursively) versus position  $n$  at a fixed time  $t/\varepsilon$ . The figure has been drawn at the instant  $t/\varepsilon = 60$ . The calculations were carried out with  $\alpha = 0.3$  and  $\beta = ar_0 = 0.5$ .

## 7.2 The nonlinear signaling problem: continuous model.

Here we return to the partial differential equation

$$\rho_t + Q'(\rho) \rho_x = 0, \quad (112)$$

subject to the boundary and initial conditions

$$\rho(0, t) = r_0, \quad t > 0; \quad \rho(x, 0) = 0, \quad x > 0. \quad (113)$$

For any  $Q(\rho)$ , the solution of this problem is given by

$$\rho(x, t) = r_0 H(t - x/\dot{s}), \quad (114)$$

where  $H$  is the Heaviside unit step function. The shock velocity  $\dot{s}$  is given by  $\dot{s} = \llbracket Q(\rho) \rrbracket / \llbracket \rho \rrbracket$  whence

$$\dot{s} = \frac{Q(r_0)}{r_0}, \quad (115)$$

where we have made use of (12)<sub>1</sub>.

The step function shown in Figure 4 is a graph of  $\rho(x, t)/r_0$  (according to (114), (115) with  $Q(\rho) = \rho + a\rho^2$ ) versus  $x/\varepsilon$  at fixed  $t/\varepsilon = 60$  for the case  $ar_0 = 0.5$ .

For the shock in the solution (114), (115), the Lax condition (43)<sub>1</sub> reduces to

$$Q'(r_0) \geq \frac{Q(r_0)}{r_0} \geq Q'(0) \quad (116)$$

in general, or to  $r_0 > 0$  for convex functions  $Q(\rho)$ ; see (44)<sub>1</sub>. Since the particular choice  $Q(\rho) = \rho + a\rho^2$ ,  $a > 0$  used in the preceding and subsequent cases is convex, the Lax condition reduces to  $r_0 > 0$  and so holds automatically.

The Lax condition (43) would be expected to suffice for uniqueness of the solution to the signaling problem for the partial differential equation (112), in the sense that if  $\rho^{(1)}$  and  $\rho^{(2)}$  are two weak solutions, each of which satisfies the Lax condition (43) at any and all shock waves, then  $\rho^{(1)} = \rho^{(2)}$ . One such solution is given by (114), (115).

### 7.3 The nonlinear signaling problem: the second-order continuous model.

We now turn to the signaling problem for the second-order continuum model governed by the nonlinear partial differential equation

$$\rho_t + Q'(\rho) \rho_x - \frac{\varepsilon}{2} \{Q'(\rho) \rho_{xx} + Q''(\rho) \rho_x^2\} = 0, \quad (117)$$

along with

$$\rho(0, t) = r_0 \text{ for } t > 0, \quad \rho(x, 0) = 0 \text{ for } x > 0; \quad (118)$$

$\rho \in C_p^2((0, \infty) \times (0, \infty))$  is required to be such that  $\rho(\cdot, t)$  is bounded on  $(0, \infty)$  for each  $t > 0$ .

#### 7.3.1 The interior approximation.

Exploiting the fact that  $\varepsilon$  is a small parameter, we view (117), (118) as a singular perturbation problem whose crudest approximation is obtained by neglecting the  $\varepsilon$ -terms in (117), which results in the problem (112), (113) discussed above and solved by (114), (115). Using the terminology of singular perturbation theory, we view (114), (115) as the “interior” approximation to the solution of the signaling problem for the full equation (117). We now ask where the “boundary layer” needed to correct this interior approximation is located. Since the interior approximation satisfies the boundary and initial conditions of the original problem, and since the signaling problem for (117) must not suffer a jump, as in (114), we would expect the boundary layer to occur near  $x = st$  in order to repair the smoothness error introduced by the shock in the interior approximation.

### 7.3.2 The boundary layer.

Returning to the differential equation (117), we let

$$\xi = x - \dot{s}t \quad (119)$$

where  $\dot{s}$  is the shock velocity (115). Under this change, (117) goes over to

$$\{Q'(\rho) - \dot{s}\} \rho_\xi + \rho_t - \frac{\varepsilon}{2} \{Q'(\rho) \rho_{\xi\xi} + Q''(\rho) \rho_\xi^2\} = 0, \quad (120)$$

where we have used the same symbol  $\rho$  in the presence of the new independent variables:  $\rho = \rho(\xi, t)$ . Taking for granted that the boundary layer occurs at  $\xi = 0$ , we tentatively assume that its effects take place on a length scale that is  $O(\varepsilon^m)$  and attempt to determine the exponent  $m$  by suitably balancing the terms in the differential equation that results from (120) under the re-scaling

$$\zeta = \xi/\varepsilon^m. \quad (121)$$

The variables  $\zeta$  and  $t$  are taken to have the ranges  $-\infty < \zeta < \infty$ ,  $t \geq 0$ . Under the re-scaling (121), equation (120) becomes

$$\varepsilon^{-m} \{Q'(\rho) - \dot{s}\} \rho_\zeta + \rho_t - \frac{1}{2} \varepsilon^{1-2m} \{Q'(\rho) \rho_{\zeta\zeta} + Q''(\rho) \rho_\zeta^2\} = 0, \quad (122)$$

where we have continued to retain the symbol  $\rho$ , despite the introduction of still another independent variable:  $\rho = \rho(\zeta, t)$ .

We note to begin with that in the *linear* case  $Q(\rho) = \rho$ , one finds from (115) that  $\dot{s} = 1$ , so that the first term in (122) is absent. In this eventuality, the only possible balance-of-terms in (122) occurs if  $m = 1/2$ , which immediately delivers the heat equation in (94).

Having dealt with it earlier, we now rule out the linear case, assuming instead that  $Q(\rho) - \dot{s}\rho$  does not vanish. It is now easy to see that only two values of  $m$  can be of interest: the first,  $m = 0$ , balances the first two terms in (122) and leaves the third term small compared to the first two. But this corresponds precisely to the first-order scalar partial differential equation (112) and hence to the interior approximation. The second choice of  $m$  — the one of interest here — is  $m = 1$ , which balances the first and third terms in (122) while leaving the second term small compared to the other two. Dropping the second term then leaves us with the desired equation for the leading approximation in the boundary layer in the nonlinear case:

$$\{Q'(\rho) - \dot{s}\} \rho_\zeta - \frac{1}{2} \{Q'(\rho) \rho_{\zeta\zeta} + Q''(\rho) \rho_\zeta^2\} = 0. \quad (123)$$

As boundary conditions at  $\zeta = \pm\infty$  for the ordinary differential equation (123), we require

$$\rho(+\infty, t) = 0 \quad \rho(-\infty, t) = r_0 , \quad (124)$$

so that the boundary layer approximation merges appropriately with the interior approximation given by the shock wave (114).

If  $\rho(\zeta, t)$  is a solution of the boundary value problem (123), (124), so is  $\rho(\zeta + b, t)$  for any constant  $b$ . To remove this translational arbitrariness, we adopt the normalization

$$\rho(0, t) = r_0/2 . \quad (125)$$

The differential equation (123) can be integrated once to give

$$Q'(\rho) \rho_\zeta - 2 \{Q(\rho) - \dot{s}\rho\} = A(t) , \quad (126)$$

where  $A(t)$  is an arbitrary function of  $t$ . Making use of the value of the shock speed given by (115), we may instead write (126) as

$$Q'(\rho) \rho_\zeta - 2 \left\{ Q(\rho) - \frac{Q(r_0)}{r_0} \rho \right\} = A(t), \quad -\infty < \zeta < \infty . \quad (127)$$

By letting  $\zeta \rightarrow +\infty$  so that  $\rho \rightarrow 0$ , or by letting  $\zeta \rightarrow -\infty$  so that  $\rho \rightarrow r_0$ , and furthermore observing that

$$Q(\rho) - \frac{Q(r_0)}{r_0} \rho = 0 \text{ when } \rho = 0 \text{ or } \rho = r_0 \quad (128)$$

since  $Q(0) = 0$ , we infer from (127) that  $A(t) = 0$ . Thus the boundary layer equation takes the final form

$$Q'(\rho) \frac{\partial \rho}{\partial \zeta} - 2 \left\{ Q(\rho) - \frac{Q(r_0)}{r_0} \rho \right\} = 0 , \quad -\infty < \zeta < \infty . \quad (129)$$

Thus in the boundary layer,  $\rho$  is determined by the boundary value problem (129), (124), (125).

### 7.3.3 An example.

Now choose the special  $Q(\rho)$  introduced previously in (107):

$$Q(\rho) = \rho + a\rho^2, \quad a > 0 . \quad (130)$$

For this choice of  $Q(\rho)$ , (129) becomes

$$(1 + 2a\rho) \frac{\partial \rho}{\partial \zeta} + 2a\rho(r_0 - \rho) = 0 . \quad (131)$$

This may be integrated to give

$$\frac{(r_0 - \rho)^{1+2\beta}}{\rho} = B \exp(2\beta\zeta) , \quad (132)$$

where  $\beta = ar_0$  as given by (110)<sub>2</sub> and  $B > 0$  is an arbitrary constant. Invoking the normalization condition (125) leads to

$$B = (r_0/2)^{2\beta} , \quad (133)$$

so that, after some simplification, (132) becomes

$$\left( \frac{r_0 - \rho}{\rho} \right)^{1/(2\beta)} (r_0 - \rho) = \frac{r_0}{2} \exp(\zeta) . \quad (134)$$

To illustrate (134), we take  $\beta = 1/2$ , obtaining

$$\frac{(r_0 - \rho)^2}{\rho} = \frac{r_0}{2} \exp(\zeta), \quad (\beta = 1/2) , \quad (135)$$

which can be solved for  $\rho/r_0$  to give

$$\frac{\rho}{r_0} = 1 - \frac{2}{1 + (1 + 8 \exp(-\zeta))^{1/2}} , \quad (\beta = 1/2) . \quad (136)$$

The right side of (136) decreases monotonically from the value 1 at  $\zeta = -\infty$  to the value of 0 at  $\zeta = +\infty$ , taking the value 1/2 at  $\zeta = 0$ .

Using (119) and (121) with  $m = 1$ , we can restore the physical variables to (134) and (136), getting

$$\left( \frac{r_0 - \rho}{\rho} \right)^{1/2\beta} (r_0 - \rho) = \frac{r_0}{2} \exp\left( \frac{x - \dot{s}t}{\varepsilon} \right) \quad (137)$$

and

$$\frac{\rho}{r_0} = 1 - \frac{2}{1 + [1 + 8 \exp\{- (x - \dot{s}t)/\varepsilon\}]^{1/2}} , \quad (\beta = 1/2) \quad (138)$$

respectively, where  $\dot{s} = Q(r_0)/r_0 = 1 + ar_0 = (1 + \beta)$ .

Figure 5 shows the graph of  $\rho/r_0$  vs.  $(x - \dot{s}t)/\varepsilon = \zeta$  for the case  $\beta = 1/2$  as given in (138).

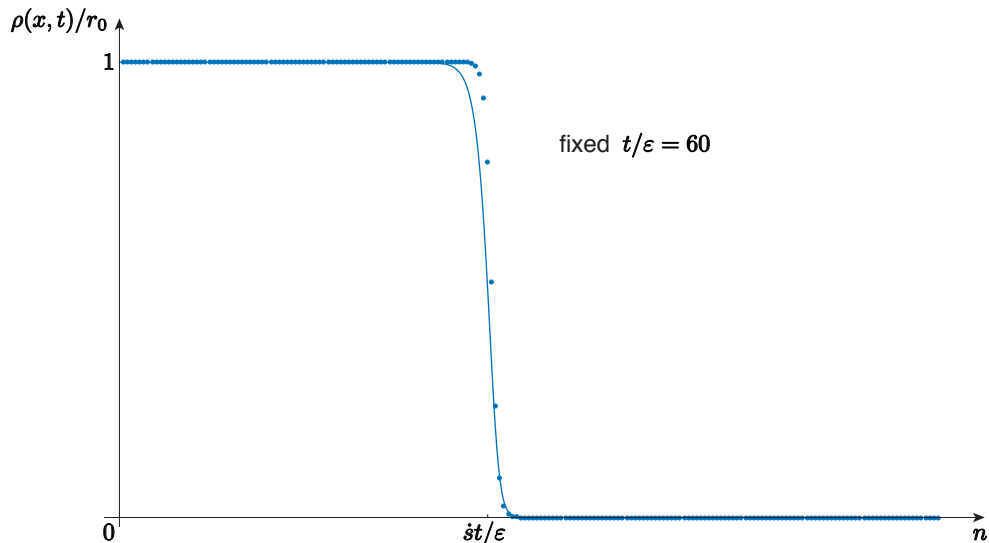


Figure 5: *The boundary layer solution of the second-order continuous nonlinear signaling problem:* The curve is a graph of the density  $\rho(x, t)/r_0$ , according to (138), versus position  $x/\varepsilon$  at a fixed time  $t/\varepsilon$ ; it has been drawn for the case  $\beta = 0.5$  and at the time  $t/\varepsilon = 60$ . The dots correspond to the solution of the nonlinear discrete problem as was displayed in Figure 4. The boundary layer solution of the second-order continuous model provides a good approximation (for this choice of parameters) to the discrete model in the nonlinear case.

**Remark:** As a final observation, we point out that choosing  $Q(\rho) = \rho$  in (123) in order to inquire about the linear case leads to a trivial result, rather than to the heat equation that we found earlier for this circumstance. Thus the result of executing the two processes under study — namely, (i) linearization and (ii) analysis near regimes of rapid change — depends on the order in which the processes are performed, suggesting that neither of the two limiting processes occurs uniformly with respect to the other.

### Acknowledgements

The authors wish to thank Srikanth Vedantam for his help with some *Mathematica* calculations and Debbie Blanchard for her help with the figures.

### References

- [1] H.B. Callen. *Thermodynamics and an Introduction to Thermostatistics*. Wiley, New York, 1985.
- [2] C. Dafermos. *Hyperbolic Conservation Laws in Continuum Physics*. Springer, New York, 1999.

- [3] W. Dreyer, M. Herrmann, and A. Mielke. Micro-Macro Transition in the Atomic Chain via Whitham's Modulation Equation. *Nonlinearity*, 19(2):471–500, 2006.
- [4] J.K. Knowles. Driving force and kinetic relations for scalar conservation laws. *Journal of Hyperbolic Differential Equations*, 4:19–38, 2007.
- [5] P.G. LeFloch. *Hyperbolic Systems of Conservation Laws: The Theory of Classical and Nonclassical Shock Waves*. Birkhäuser, Basel, 2002.
- [6] M.J. Lighthill and G.B. Whitham. On Kinematic Waves .2. A Theory of Traffic Flow on Long Crowded Roads. *Proceedings of the Royal Society of London Series A-Mathematical and Physical Sciences*, 229(1178):317–345, 1955.
- [7] P. Purohit. *Dynamics of Phase Transitions in Strings, Beams, and Atomic Chains*. Ph.D. dissertation, California Institute of Technology, Pasadena, CA, November 2001.
- [8] P. Rosenau. Dynamics of Dense Lattices. *Physical Review B*, 36(11):5868–5876, 1987.
- [9] C. Truesdell. *Rational Thermodynamics*. McGraw-Hill, New York, 1969.
- [10] G.B. Whitham. *Linear and Nonlinear Waves*. Wiley, New York, 1974.