Convergence of the relaxation approximation to a scalar nonlinear hyperbolic equation arising in chromatography

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Abstract

For a single nonlinear hyperbolic equation, we prove the convergence of the solution to the so-called "local-equilibrium relaxation system" to that of the original conservation law, when the relaxation parameter tends to zero. Our study is motivated by a model arising in the theory of gaseous chromatography, where the flux function appearing in the conservation law is obtained from a thermodynamical assumption of local equilibrium. The relaxation of this assumption naturally leads to a chemical kinetic equation, in which the (small) relaxation parameter is the inverse of the reaction rate. The convergence of such zero-relaxation limits has been studied in a very general framework by G.Q.Chen, C.D.Levermore and T.P.Liu [15, 3, 4], and most of the results we present here are in fact already contained in these papers. However we deal here with a particular case and therefore, assuming of course that the so-called "subcharacteristic condition" introduced by Liu [15] is satisfied, we can give very direct and explicit relations between the entropies of the limit equation and those of the relaxed system. The latter is also semi-linear, which sligthly simplifies the proof of convergence by compensated compactness in section 2. Since our primary interest here is the above-mentioned physical problem, we have tried to make the mathematical part of this paper self-contained. We conclude by applying the above ideas to two natural relaxations in this gaseous chromatography model. The "subcharacteristic condition" is then equivalent to the strict monotonicity of the function f appearing in the equilibrium relation.

1 Introduction

Let us consider the Cauchy problem for a scalar nonlinear conservation law in one space dimension:

$$\begin{aligned} &\partial_t u + \partial_x f(u) = 0 \\ &u(x,0) = u_0(x) \quad x \in I\!R. \end{aligned} \tag{1.1}$$

It is a natural idea to try to replace (1.1) by the relaxed system:

$$\begin{aligned} &\partial_t u^\epsilon + \partial_x v^\epsilon = 0 \\ &\partial_t v^\epsilon + a^2 \partial_x u^\epsilon = \tfrac{1}{\epsilon}(f(u^\epsilon) - v^\epsilon) \end{aligned} \tag{1.2}$$

where a^2 is a scalar parameter, with the initial condition:

$$u^\epsilon(x,0) = u_0(x), \quad v^\epsilon(x,0) = f(u_0(x)).$$

The system (1.2) has the advantage of being linear, but it is not clear a-priori wether it induces a singular limit. Relaxed systems similar to (1.2) often arise from physical considerations, and are the object of much current research. For theoretical results on the convergence of the relaxation process in a very general setting we refer the reader to [15, 3]. Reference [4] contains the proof of convergence for a particular model arising in viscoelasticity, and numerical algorithms for relaxed systems are studied in [12, 14, 13]. A simple computation shows that the first-order approximation to (1.2), obtained by a formal Chapman-Enskog expansion, is given by:

$$\partial_t u + \partial_x f(u) = \epsilon \partial_x[(a^2 - f'(u)^2)\partial_x u], \tag{1.3}$$

and is thus dissipative provided the stability condition:

$$-a < f'(u) < a \tag{1.4}$$

holds. This condition was introduced by Liu [15], and expresses the fact the characteristic speeds for the relaxed system (1.2) are greater than those for the original equation (1.1). It will allow for the extension of entropy-flux pairs (η^*, q^*) for (1.1) to entropy-flux pairs for (1.2) which coincide with (η^*, q^*) on the equilibrium curve $\{v = f(u)\}$. The convergence result may be stated as follows:

Theorem 1.1 *Suppose that the initial data is bounded. Let $a > 0$ be chosen in such a way that the condition (1.4) is satisfied for u_0. Then:*

- *for any $\epsilon > 0$, the relaxed system (1.2) has a unique solution (u^ϵ, v^ϵ) defined for all time;*
- *suppose that there is no interval on which the flux function f is affine. Then for any $p \in]0, \infty[$ and $T \in [0, \infty[$ we have the strong convergences in $L^p(I\!\!R \times [0,T])$*

  $$u^\epsilon \to u, \quad v^\epsilon \to f(u),$$

  when $\epsilon \to 0^+$, where u is the (unique) entropy solution to the original equation (1.1).

A more general result is proved in [3]. Note that we might have considered a relaxed system with initial data for v^ϵ different from $f(u_0)$. Such a choice for the initial data would create an initial layer at $t = 0$ for v^ϵ, but the convergence result for u^ϵ would still hold true. The remainder of this section is devoted to the existence of (u^ϵ, v^ϵ) for fixed $\epsilon > 0$. Section 2 contains the proof of the convergence result, and in section 3 we present the application of this result to the chromatography model which motivated our study. The system (1.2) has the two characteristic speeds $\pm a$, and the associated Riemann invariants are

$$w_1 = v + au, \quad w_2 = v - au.$$

Thus, for any choice of the constants c_1, c_1', c_2, c_2', the region $\mathcal{R}$ defined in the $u-v$ plane by

$$\mathcal{R} = \{(u,v) : c_1 \leq w_1 \leq c_1';\, c_2 \leq w_2 \leq c_2'\} \tag{1.5}$$

is a convex invariant region (see [7]). Since it is bounded, this yields an L^∞ bound on the solution (u^ϵ, v^ϵ). Moreover the system (1.2) is semilinear. Therefore, if the constants c_1, c_1', c_2, c_2' are chosen in such a way that the initial data $u_0, f(u_0)$ belong to $\mathcal{R}$, then the solution (u^ϵ, v^ϵ) is globally defined, and belongs to $\mathcal{R}$, for all time. One can give a geometric interpretation of the condition (1.4): if the initial data u_0 satisfies $u_1 \leq u_0(x) \leq u_2$ for all x, let us define the constants c_1, c_1', c_2, c_2' by:

$$\begin{array}{l} f(u_1) - au_1 = c_2',\ f(u_1) + au_1 = c_1, \\ f(u_2) - au_2 = c_2,\ f(u_2) + au_2 = c_1'. \end{array} \tag{1.6}$$

Let $\mathcal{R}$ be the region defined by (1.5) with this particular choice of the constants c_1, c_1', c_2, c_2'; the equalities (1.6) mean that the leftmost and rightmost corners of $\mathcal{R}$ belong to the graph of f; for any $u \in [u_1, u_2]$, we have from (1.4):

$$f(u_1) - a(u - u_1) \leq f(u) \leq f(u_1) + a(u - u_1)$$

so that

$$c_1 = f(u_1) + au_1 \leq f(u) + au, \quad f(u) - au \leq f(u_1) - au_1 = c_2',$$

and similarly with c_2 and c_1', so that $(u, f(u)) \in \mathcal{R}$. In other words, (1.4) ensures that the portion of the graph of f corresponding to $u_1 \leq u \leq u_2$ is entirely contained in $\mathcal{R}$. Of course this invariant region $\mathcal{R}$ does not depend on ϵ, and therefore:

$$\forall \epsilon > 0,\, \forall x \in I\!R,\, \forall t \geq 0: \quad (u^\epsilon(x,t), v^\epsilon(x,t)) \in \mathcal{R} \tag{1.7}$$

2 The convergence of the relaxation process

The proof of the second assertion of theorem (1.1) will be done in four lemmas. It is based as in [4, 3] on the use of compensated compactness, via the construction of particular entropy-flux pairs for the system (1.2). For general background on compensated compactness we refer the reader for instance to [10, 11, 8]. >From here on, we will assume u_0 to be bounded:

$$u_1 \leq u_0(x) \leq u_2 \quad \forall x \in I\!R,$$

the region $\mathcal{R}$ will be defined as in the preceding section (i.e., via (1.6) and (1.5)), and we will assume the subcharacteristic condition to hold true:

$$\forall u \in [u_1, u_2]: \quad -a < f'(u) < a. \tag{2.1}$$

The first lemma shows how to extend arbitrarily given entropy-flux pairs (η^*, q^*) for the original equation to entropy-flux pairs for the relaxed system which coincide with (η^*, q^*) on the equilibrium curve. The explicit construction of a particular pair is given in [6]

Lemma 2.1 *Let (η^*, q^*) be an entropy-flux pair for the equation (1.1); then if the subcharacteristic condition (2.1) is satisfied, there exists a unique entropy-flux pair (η, q) for the relaxed system (1.2) satisfying:*

$$\forall u \in [u_1, u_2]: \quad \eta(u, f(u)) = \eta^*(u),\, q(u, f(u)) = q^*(u), \tag{2.2}$$

and this pair also satisfies:

$$\forall u \in [u_1, u_2]: \quad \eta_v(u, f(u)) = 0, \tag{2.3}$$

$$\min_{\mathcal{R}} \eta_{vv} \geq K \min_{[u_1,u_2]} \frac{d^2\eta^*}{d^2u} \tag{2.4}$$

for some positive constant K. In particular η is uniformly convex if the same property holds for the original entropy η^*.

Proof.
An entropy-flux pair (η, q) for the relaxed system (1.2) must satisfy

$$a^2\eta_v = q_u, \quad \eta_u = q_v,$$

so that η must satisfy the wave equation

$$\eta_{uu} = a^2\eta_{vv}.$$

Let us remark that the equilibrium curve $\{(u, v) : v = f(u)\}$ is not characteristic for the Cauchy problem associated to this wave equation, if and only if we have $f'(u)^2 \neq a^2$ for all u. In other words, the condition (2.1) garantees that the equilibrium curve is space-like for this wave equation, so that prescribing data on this curve leads to a well-posed Cauchy problem. In this case η must take the form:

$$\eta(u, v) = \eta_1(v + au) + \eta_2(v - au),$$

and in view of the extension conditions (2.2) we must have:

$$\begin{array}{l} \eta_1(f(u) + au) + \eta_2(f(u) - au) = \eta^*(u), \\ a\eta_1(f(u) + au) - a\eta_2(f(u) - au) = q^*(u), \end{array} \tag{2.5}$$

or equivalently:

$$\begin{array}{l} 2a\eta_1(f(u) + au) = a\eta^*(u) + q^*(u), \\ -2a\eta_2(f(u) - au) = -a\eta^*(u) + q^*(u). \end{array} \tag{2.6}$$

>From the condition (2.1) we see that the functions $u \mapsto f(u) \pm au$ are strictly increasing on the interval $[u_1, u_2]$, in such a way that the preceding system uniquely defines the functions η_1 and η_2. Differentiating (2.5) with respect to u we obtain:

$$(f'(u) + a)\eta_1'(f(u) + au) + (f'(u) - a)\eta_2'(f(u) - au) = \eta^{*\prime}(u), \tag{2.7}$$

$$a[(f'(u) + a)\eta_1'(f(u) + au) - (f'(u) - a)\eta_2'(f(u) - au)] = q^{*\prime}(u), \tag{2.8}$$

i.e.:

$$(f'(u)^2 - a^2)[\eta_1'(f(u) + au) + \eta_2'(f(u) - au)] = 0,$$

which gives (2.3). Combining this last relation to (2.7) we obtain:

$$2a\eta_1'(f(u) + au) = \eta^{*\prime}(u),$$

and differentiating this last relation yields:

$$2a(f'(u) + a)\eta_1''(f(u) + au) = \eta^{*\prime\prime}(u).$$

The inequality (2.4) now follows, in view of the condition (2.1), and the surjectivity of the function $u \mapsto f(u) + au$. This concludes the proof of Lemma 2.1. Let us mention that the explicit construction of a particular pair may be found in [6]. The next lemma gives an energy estimate for the deviation from local equilibrium in the relaxed system:

Lemma 2.2 *Let (u^ϵ, v^ϵ) be the (unique) solution to the relaxed system (1.2) obtained in section 1, and for fixed $T > 0$ let Q_T denote $I\!R \times [0, T]$; then we have:*

$$||f(u^\epsilon) - v^\epsilon||_{L^2(Q_T)} = \mathcal{O}(\sqrt{\epsilon}).$$

Proof.
Let (η, q) be an entropy-flux pair for the relaxed system, satisfying the following inequalities:

$$\eta \geq 0 \quad \text{in} \quad \mathcal{R} \tag{2.9}$$

$$C := \min_{\mathcal{R}} \eta_{vv} > 0, \quad \eta_v(u, f(u)) = 0 \quad \forall u \in [u_1, u_2]; \tag{2.10}$$

such a pair may be obtained by applying Lemma 2.11 to a strictly convex entropy η^*, and adding if necessary an appropriate constant to the resulting η. Multiplying the first equality in (1.2) by $\eta_u(u^\epsilon, v^\epsilon)$, the second by $\eta_v(u^\epsilon, v^\epsilon)$ and adding, we obtain:

$$\partial_t \eta(u^\epsilon, v^\epsilon) + \partial_x q(u^\epsilon, v^\epsilon) = \frac{1}{\epsilon}\eta_v(u^\epsilon, v^\epsilon)(f(u^\epsilon) - v^\epsilon).$$

Integrating over Q_T we obtain:

$$\int_{I\!R} \eta(u^\epsilon(x,T), v^\epsilon(x,T))\, dx - \int_{I\!R} \eta(u^0(x), v^0(x))\, dx = \frac{1}{\epsilon}\int_{Q_T} \eta_v(u^\epsilon, v^\epsilon)(f(u^\epsilon) - v^\epsilon)\, dt\, dx,$$

and therefore:

$$\frac{1}{\epsilon}\int_{Q_T} \eta_v(u^\epsilon, v^\epsilon)(v^\epsilon - f(u^\epsilon))\, dt\, dx \leq \int_{I\!R} \eta(u^0(x), v^0(x))\, dx. \tag{2.11}$$

For $(u^\epsilon, v^\epsilon) \in \mathcal{R}$ we have:

$$\eta_v(u^\epsilon, v^\epsilon) = (v^\epsilon - f(u^\epsilon))\eta_{vv}(\alpha_\epsilon, \beta_\epsilon)$$

for some $(\alpha_\epsilon, \beta_\epsilon) \in \mathcal{R}$ (since $\mathcal{R}$ is convex), and thus:

$$\eta_v(u^\epsilon, v^\epsilon)(v^\epsilon - f(u^\epsilon)) \geq C|v^\epsilon - f(u^\epsilon)|^2.$$

This last inequality combined to (2.11) shows that the quantity $\frac{1}{\sqrt{\epsilon}}(v^\epsilon - f(u^\epsilon))$ is bounded in $L^2(Q_T)$ independently of ϵ.

Lemma 2.3 *Let us define g by $g(u) := \int_0^u (f')^2(s)\, ds$. Let (u^ϵ, v^ϵ) be the solution to the relaxed system. Then for the pair (f, g) or more generally for any entropy-flux pair (η^*, q^*) of (1.1) the sequences*

$$\alpha^\epsilon := \partial_t u^\epsilon + \partial_x f(u^\epsilon), \tag{2.12}$$

and

$$\beta^\epsilon := \partial_t \eta^*(u^\epsilon) + \partial_x q^*(u^\epsilon) \tag{2.13}$$

lie in a strongly compact subset of the negative Sobolev space $H^{-1}_{loc}(Q_T)$. Moreover the limit of (a subsequence) (β^ϵ) is nonnegative if η^* is convex.

Proof.
First we have

$$\alpha^\epsilon := \partial_t u^\epsilon + \partial_x f(u^\epsilon) = \partial_t u^\epsilon + \partial_x v^\epsilon + \partial_x(f(u^\epsilon) - v^\epsilon), \tag{2.14}$$

which implies the compactness of (α^ϵ) by Lemma 2.2. By Lemma 2.1 we extend the pair (η^*, q^*) to the entropy-flux pair $(\eta, q) := (f, g)$ for the relaxed system, to get

$$\begin{array}{rcl} \beta^\epsilon := \partial_t \eta(u^\epsilon, f(u^\epsilon)) + \partial_x q(u^\epsilon, f(u^\epsilon)) & = & \partial_t \eta(u^\epsilon, v^\epsilon) + \partial_x q(u^\epsilon, v^\epsilon) \\ +\partial_t(\eta(u^\epsilon, f(u^\epsilon)) - \eta(u^\epsilon, v^\epsilon)) & + & \partial_x q(u^\epsilon, f(u^\epsilon)) - \partial_x q(u^\epsilon, v^\epsilon)). \end{array} \tag{2.15}$$

By Lemma 2.2 the last two quantities are strongly compact in H^{-1} since their norms in this space are of order $\epsilon^{1/2}$. On the other hand the first term in the right-hand side of (2.14) satisfies

$$\partial_t \eta(u^\epsilon, v^\epsilon) + \partial_x q(u^\epsilon, v^\epsilon) = \frac{1}{\epsilon}\eta_v(u^\epsilon, v^\epsilon)(f(u^\epsilon) - v^\epsilon) \tag{2.16}$$

which is bounded in L^1 by Lemma 2.2. The result follows from Murat's Lemma [9]. Moreover we see from (2.3) and (2.4) that the right-hand side of (2.16) is nonnegative if η^* is convex.

Lemma 2.4 *Assume there is no interval on which f is affine. Then for any finite p we have, at least at least for a subsequence,*

$$(u^\epsilon, v^\epsilon) \to (u, f(u)) \; in L^p(Q_T) \times L^2(Q_T) \tag{2.17}$$

where u is the unique admissible weak solution to (1.1).

Proof.
Let $\nu_{x,t}$ denote the Young measure associated to the sequence (u^ϵ). Using the div-curl Lemma we obtain almost everywhere and for any k in $I\!R$

$$\begin{array}{rl} < \nu_{x,t}, (s-k)(g(s)-g(k)) - (f(s)-f(k))^2 > & = \\ < \nu_{x,t}, s-k >< \nu_{x,t}, g(s)-g(k) > & -(< \nu_{x,t}, f(s)-f(k) >)^2. \end{array} \tag{2.18}$$

Choosing now $k =< \nu_{x,t}, s >= u(x,t)$, we see that the right-hand side of (2.18) is nonpositive. On the other hand, $\nu_{x,t}$ is nonnegative and we recall that $g' = (f')^2$. Therefore the left-hand side of (2.15) is nonnegative, since by Cauchy-Schwarz inequality

$$(f(s) - f(k))^2 = (\int_k^s f'(y)dy)2 \leq (s-k)(g(s)-g(k)). \tag{2.19}$$

We also remark that the equality in (2.19) is only possible either if $s = k$ or if f is affine on the interval $[k, s]$. We have thus proved that the left-hand side of (2.18) vanishes. Consequently the support of the Young measure $\nu_{x,t}$ satisfies almost everywhere

$$\mathrm{supp}(\nu_{x,t}) \in \{s \in I\!R / h(x,t,s) := (g(s) - g(k))^2 - (s-k)(f(s) - f(k)) = 0\}$$

In any case that implies

$$< \nu_{x,t}, f(s) - f(k) >= 0.$$

In other words, even if the convergence were weak we would have

$$f(u^\epsilon) \to f(u) \; \mathrm{in} L^\infty weak - star,$$

and therefore

$$v^\epsilon \to f(u) \; \mathrm{in} L^\infty weak - star,$$

since

$$v^\epsilon - f(u^\epsilon) \to 0 \mathrm{in} L^2$$

(strongly). Here, since there is no interval on which f is affine, then by (2.19) $\nu_{x,t}$ is a family of delta-functions. Therefore

$$u^\epsilon \to u \ \mathrm{in} L^p$$

for any finite p, and similarly

$$v_\epsilon \to f(u).$$

Finally, this strong convergence implies by Lemma 2.3 that u satisfies the Lax entropy condition and therefore is the unique admissible weak solution to (1.1).

3 Application to gaseous chromatography

3.1 Introduction and the simplest relaxation

In this section we present a physical model which motivated our study, and to which the general framework of section 1 may be applied. The physical situation we are interested in is gaseous chromatography. Let us consider a one-dimensionnal pipe filled with solid porous material; assume that a gas is injected in this column, and is not in chemical equilibrium with the solid. For simplicity we will assume that the chemical reactions between the gas and the solid amount to the exchange of one chemical species; we will denote by m_f, m_s respectively, the concentrations of this species within the gas and the solid. The other physical parameters are p, the porosity of the column ($0 < p < 1$), and c, the velocity of the gas. These two parameters will be taken constant for simplicity. The mass conservation equation for the chemical species then reads:

$$p\partial_t m_f + (1-p)\partial_t m_s + pc\partial_x m_f = 0. \tag{3.1}$$

Another equation is needed to compute the time evolution of the quantities m_f, m_s. The traditional assumption of"local equilibrium" asserts that the chemical kinetics are significantly faster than the hydrodynamical effects, so that the two phases can be assumed to be in local chemical equilibrium at any point. The chemical potentials of the species in the two phases will therefore be equal:

$$\mu_f(m_f) = \mu_s(m_s),$$

which yields an explicit relation (the so-called"isotherm"):

$$m_f = f(m_s). \tag{3.2}$$

Combining (3.1) and (3.2) we obtain a nonlinear transport equation which can be used to compute the functions $m_f(x,t)$ and $m_s(x,t)$. For more details on this model we refer the reader to [2, 1]. It is clear from physical considerations that the function f should be strictly increasing, and so (3.1)-(3.2) may be recast in the form of a standard hyperbolic equation:

$$\partial_t m_s + \partial_x \phi(m_s) = 0,$$

where the function ϕ satisfies:

$$\phi'(m_s) = \frac{pcf'(m_s)}{1-p+pf'(m_s)}$$

Our convergence result may then be applied to the relaxed system:

$$\begin{cases} \partial_t m_s^\epsilon + \partial_x m_t^\epsilon = 0 \\ \partial_t m_t^\epsilon + a^2 \partial_x m_s^\epsilon = \dfrac{1}{\epsilon}(\phi(m_s^\epsilon) - m_t^\epsilon). \end{cases} \tag{3.3}$$

However the physical meaning of the function ϕ is not clear (only ϕ' can be interpreted as a propagation velocity), in such a way that this relaxation may seem somewhat artificial; in the next subsection we present a more physical relaxation, and briefly indicate how the method of proof of the first section may be used to cover this case.

3.2 The relaxation based on particle derivatives

Let us set $u = pm_f + (1-p)m_s$ (the total concentration), and $v = m_f$. The problem may then be rewritten:

$$\begin{cases} \partial_t u + pc\partial_x v = 0 \\ v = f(\dfrac{u}{1-p} - \dfrac{p}{1-p}v). \end{cases} \tag{3.4}$$

The local equilibrium curve given in the $(m_s - m_f)$ plane by (3.2) is now represented in the $u-v$ plane by the second equation of (3.4); a natural way to relax this local equilibrium assumption is to replace this equality by a chemical kinetic equation specifying the material derivative of v (see [5]). This leads to the new relaxed system:

$$\begin{cases} \partial_t u + pc\partial_x v = 0 \\ \partial_t v + c\partial_x v = \dfrac{1}{\epsilon}[f(\dfrac{u}{1-p} - \dfrac{p}{1-p}v) - v]. \end{cases} \tag{3.5}$$

This system is not of the same type as the system (1.2); however we can briefly sketch how our method of proof may be applied here: let us assume that the equilibrium curve may be locally parametrized by a function $v = V^*(u)$; writing a Chapman-Enskog expansion for v in the form:

$$v = V^*(u) + \epsilon v_1(u) + \cdots,$$

a little algebra shows that the first order approximation to (3.5) is:

$$\partial_t u + pc\partial_x[V^*(u) - \epsilon c(1-p)^2 \frac{f'(w)}{(1-p+pf'(w))^3}\partial_x u] = 0,$$

where for convenience we have set

$$w = \frac{u - pv}{1-p}.$$

This equation is dissipative since f is strictly increasing. One can easily check that any given entropy pair for the equation (3.4) may be extended to yield an entropy pair for the system (3.5), the two pairs coinciding on the equilibrium curve. The key point here, which replaces the subcharacteristic condition of section 1, is the strict monotonicity of f. Again it can be checked that for this extension, the $v-$derivative of the entropy vanishes on the equilibrium curve, and this allows one to estimate the entropy production, thus getting the required compactness.

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