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Transition to Detonation in Dynamic Phase Changes

LEV TRUSKINOVSKY

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Abstract

Subsonically propagating phase boundaries (kinks) can be modelled by material discontinuities which satisfy integral conservation laws plus an additional jump condition governing the phase-change kinetics. The necessity of an additional jump condition distinguishes kinks from the conventional shocks which satisfy the Lax criterion. We study stability of kinks with respect to the breakup (splitting) into a sequence of waves. We assume that all conventional shocks are admissible and that admissible kinks are selected by a prescribed kinetic relation. As we show, regardless of a particular choice of the kinetic relation, sufficiently fast-phase boundaries are unstable. The mode of instability includes an emission of a centered Riemann wave followed by a sonic shock (Chapman-Jouguet type phase boundary).

1. Introduction

The motivation for this study arises from experiments on martensitic phase transitions. The experiments reveal that a martensitic interface moves in a direction normal to itself when sufficient driving force is available. Since the work of FÖRSTER & SCHEIL (1940), it has been common to draw a distinction between fast (*umklapp*) and slow (*schiebung*) martensitic transformations (cf. NISHIYAMA (1978)). The fast interface moves at a velocity close to that of a corresponding elastic wave, while the slow growth can be easily observed with an optical microscope; under some circumstances the transition to the umklapp regime is accompanied by audible "clicks", which signify a "burst of transformation". In the physics literature, it has often been assumed that the difference in speeds reflects a fundamental difference in the *mechanism* of growth and is associated with some kind of instability in the *interface kinetics* (GRUJICIC et al. (1985), YU & CLAPP (1989)). In this paper we discuss a different interpretation of this phenomenon as an *inertia-driven* transition from one dynamical regime to the other, which is somewhat similar to the transition from deflagration to detonation.

We focus on the elastodynamical aspect of the phenomenon. Since the seminal paper of ERICKSEN (1975) it has been widely recognized that nonlinear elasticity is amenable to the modelling of equilibrium phase transformations provided that the governing equations lose ellipticity for a certain range of strains. After the papers of DAFERMOS (1969, 1973), KNOWLES (1979) and JAMES (1980) it has also become clear that the corresponding dynamic theory admits the propagation of discontinuities, simulating highly localized phase transitions. At the same time, the initial-value problem was found to be generically ill-posed, which results in a dramatic lack of uniqueness. It became common to view this nonuniqueness as arising from a constitutive deficiency in the theory, reflecting the need to specify additional pieces of constitutive information (cf. TRUSKINOVSKY (1982), SLEMROD (1983), ABEYARATNE & KNOWLES (1987), GURTIN & STRUTHERS (1990)). Several criteria were used to pick out physically admissible solutions (cf., e.g., DAFERMOS (1973), SHEARER (1982), HATTORI (1986), PENCE (1986), PEGO (1987), HSIAO (1991)). Contrary to the theory of conventional shock waves, the proposed admissibility criteria allow subsonic discontinuities singled out by an additional jump relation governing the phase-change kinetics. Following TRUSKINOVSKY (1993 a) we call these discontinuities *kinks*. The necessity for an additional jump condition distinguishes kinks from the conventional shocks which satisfy the *Lax criterion* (LAX (1971)).

In this paper we investigate the condition of instability of subsonic phase boundaries against *breakup* into a sequence of different waves. We adopt the simplest one-dimensional isothermal model of phase-transformation dynamics described by a nonlinear wave equation with a nonmonotone stress-strain relation. Subsonically propagating phase boundaries (kinks) are modelled by material discontinuities which satisfy integral conservation laws. We assume that all conventional shocks are admissible and that admissible kinks are selected by a prescribed kinetic relation (of the form discussed by TRUSKINOVSKY (1987) and ABEYARATNE & KNOWLES (1990), among others).

We derive a characteristic inequality which governs the stability of the kink. Then we show that sufficiently fast kinks are unstable, regardless of the particular choice of the kinetic relation. The instability arises from the nonuniqueness of the solution of the Riemann problem. A similar type of nonuniqueness has been discussed by SHEARER (1986), ABEYARATNE & KNOWLES (1991 a) and PENCE (1992) in the context of dynamic phase transitions and has long been known for classical shock waves (cf. MENIKOFF & PLOHR (1989), FOWLES (1993)). The mode of instability contains a forward-moving Riemann wave (precursor) with an attached sonic detonation wave at the rear and a backward moving classical shock wave.

It is interesting that the above mechanism of instability is not possible if only those kinks and conventional shocks which are selected by the *viscosity-capillarity criterion* (cf. TRUSKINOVSKY (1982), SLEMROD (1983)) are considered admissible. The uniqueness of the Riemann problem in this case (cf. FAN & SLEMROD (1991), SHEARER & YANG (1992)) originates from the surprising fact that the class of conventional shocks admissible by the viscosity-capillarity criterion is much narrower than the class of shocks admitted by the Lax criterion.

In Section 2, we describe an elastodynamic model with a nonmonotone stress-strain relation and specify a single-wave solution whose stability we plan to examine. The split-wave solution is discussed in Section 3. The main theorem, showing the existence of an alternative solution, is formulated and proved in Section 4. In Section 5, we examine the properties of the alternative solution; in particular, we observe that the entropy production rate may be either larger or smaller for the split waves than for the single wave solution. The implications of the viscosity-capillarity model are considered in Section 6. Finally, in Section 7 we give a heuristic discussion of stability for the single wave solution.

2. Preliminaries

The nonlinear wave equation

$$\rho y_{tt} = \sigma'(y_x)\, y_{xx} \tag{2.1}$$

with nonmonotone $\sigma(y_x)$ constitutes the simplest fully dynamical model for studying *isothermal* phase transitions. Here $y(x, t)$ denotes the displacement at time t of a reference point x. A prime indicates the derivative with respect to y_x, while subscripts x and t stand for the corresponding partial derivatives. Although the isothermal model is hardly adequate for the description of fast dynamic phase changes, it may be viewed as a natural starting point.

With the reference mass density fixed at $\rho = 1$, (2.1) generates the associated first-order system of conservation laws for the functions $u = y_x - 1$, $v = y_t$:

$$\begin{aligned} u_t &= v_x, \\ v_t &= \sigma_x. \end{aligned} \tag{2.2}$$

The constitutive function

$$\sigma = \sigma(u) \tag{2.3}$$

delivers the stress corresponding to the strain u. It is assumed that the smooth function $\sigma(u)$ takes the form indicated in Fig. 1 and satisfies the following conditions

$$\begin{gathered} \sigma' > 0, \quad \sigma'' < 0 \quad \text{if } u < \alpha, \\ \sigma' > 0, \quad \sigma'' > 0 \quad \text{if } u > \beta, \\ \sigma' \leqq 0 \quad \text{if } \alpha \leqq u \leqq \beta. \end{gathered} \tag{2.4}$$

Different phases correspond to the maximal intervals of the *monotone* behavior of $\sigma(u)$. Assume that the material is in the α phase if $u \leqq \alpha$ and in the β phase if $u \geqq \beta$. Let $u = a \leqq \alpha$ be a given point in the α-phase. When

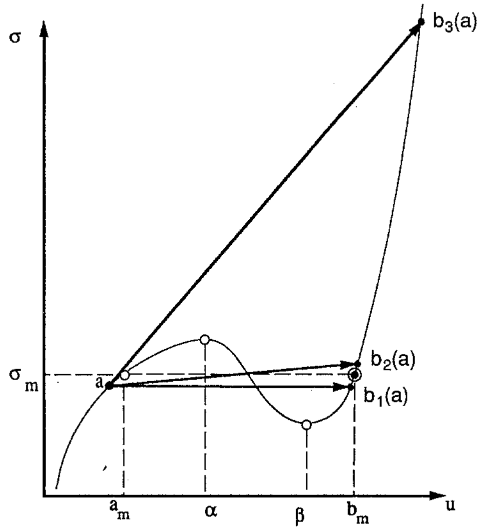

Fig. 1. A typical stress-strain curve for an elastic material which admits phase change. The chord $a \to b_3$ is tangent to $\sigma(u)$ at $u = a$ (Chapman-Jouguet regime). The chord $a \to b_1$ is horizontal. The horizontal dashed line corresponds to the Maxwell stress. The chord $a \to b_2$ cuts equal areas from the curve $\sigma(u)$ (Maxwell regime).

it exists, we let $u = b_1(a) \geqq \beta$ be the point in the β-phase at which

$$\sigma(b_1(a)) = \sigma(a). \tag{2.5}$$

Similarly, we denote by $b_2(a)$ the point in the β-phase at which

$$\int_a^{b_2(a)} \sigma \, du = \frac{\sigma(a) + \sigma(b_2(a))}{2} (b_2(a) - a), \tag{2.6}$$

again provided that such a point exists (see Fig. 1). If $a = a_m$ is a point in the α-phase such that

$$b_1(a_m) = b_2(a_m) \stackrel{\text{def}}{=} b_m,$$

we call $\sigma_m = \sigma(a_m) = \sigma(b_m)$ the *Maxwell stress*. We call $c(u) \stackrel{\text{def}}{=} \sqrt{\sigma'(u)}$ the local characteristic (sound) velocity for the hyperbolic domain where $\sigma' \geqq 0$ and introduce the notation $b_3(a)$ for the point in the β-phase (if such a point exists) which satisfies the equation

$$\sqrt{\frac{\sigma(b_3(a)) - \sigma(a)}{b_3(a) - a}} = c(a). \tag{2.7}$$

For the sake of definiteness, assume that (2.7) has a unique solution defined for all $a \leqq \alpha$ (see Fig. 1). This is true, for instance, in the case when $\sigma(u)$ is a cubic polynomial:

$$\sigma(u) = \sigma_m + k(u - a_m)(u - b_m)\left(u - \frac{a_m + b_m}{2}\right). \tag{2.8}$$

In this particular case, one can easily see that the graphs of $b = b_2(a)$ and $b = b_3(a)$ are represented by segments of straight lines, while the graph of $b = b_1(a)$ is an arc of an ellipse. The three functions, defined by (2.5), (2.6) and (2.7) are illustrated in Fig. 1 (see also Fig. 5). The inverse of these functions were considered earlier in PENCE (1992).

Since $\sigma(u)$ is a nonmonotone function, the system (2.2) is of mixed type and therefore the initial-value problem is ill-posed. We shall be particularly interested in the initial data for the *Riemann problem*,

$$u(x, 0), v(x, 0) = \begin{cases} u_-, v_-, & x < 0, \\ u_+, v_+, & x \geqq 0 \end{cases} \tag{2.9}$$

where u_+, u_-, v_+, v_- are constants. Since both the system (2.2) and the data (2.9) are invariant under a uniform stretching of the variables x and t, consider a centered solution depending on $\xi = x/t$ alone. Such a solution contains a family of waves that emanate from the origin and propagate with constant speeds. It includes constant states joined by *centered Riemann waves* or *jump discontinuities.*

A *centered Riemann wave* is a differentiable solution of (2.2) of the form $u(\xi)$, $v(\xi)$, in which one of the Riemann invariants

$$v \mp \int^{u} c(\mu)\, d\mu \tag{2.10}$$

is constant; the ξ dependence is then implicitly given by

$$\xi = \pm c(u)\,. \tag{2.11}$$

In particular, for the forward moving "fan" of the form (2.10), (2.11), the constant states on the right (u_+, v_+) and on the left (u_-, v_-) that are connected by the wave satisfy

$$v_- = v_+ - \int_{u_+}^{u_-} c(u)\, du\,. \tag{2.12}$$

For the material under consideration, the centered Riemann wave may correspond to either compression or rarefaction. That is, $u_- > u_+$ if $\sigma''(u) < 0$ for $u \in (u_+, u_-)$, and $u_- < u_+$ if $\sigma''(u) > 0$ for $u \in (u_-, u_+)$. It is clear that Riemann waves are defined only in the hyperbolic region $\sigma'(u) \geqq 0$.

A *jump discontinuity* is a pair of functions (u, v) of the form

$$(u, v)(x, t) = \begin{cases} u_+, v_+, & x > Dt, \\ u_-, v_-, & x \leqq Dt \end{cases}$$

which satisfy the Rankine-Hugoniot jump conditions

$$\begin{aligned} D(v_+ - v_-) + (\sigma_+ - \sigma_-) &= 0, \\ D(u_+ - u_-) + (v_+ - v_-) &= 0. \end{aligned} \tag{2.13}$$

Here D is the velocity of the discontinuity, $\sigma_+ = \sigma(u_+)$ and $\sigma_- = \sigma(u_-)$. Assuming $u_+ \neq u_-$, we solve (2.13) for D and obtain for the forward and backward moving discontinuity

$$D = \pm \sqrt{\frac{\sigma_+ - \sigma_-}{u_+ - u_-}}. \tag{2.14}$$

The right and left particle velocities are then related by

$$v_+ - v_- = \mp \sqrt{(\sigma_+ - \sigma_-)(u_+ - u_-)}\,. \tag{2.15}$$

In an attempt to single out physically meaningful discontinuities, several *admissibility criteria*, which we briefly discuss in the rest of this section, have been suggested (cf. LAX (1971), LIU (1981), DAFERMOS (1985), FAN & SLEMROD (1991), HATTORI & MISCHAIKOW (1991) and the literature cited therein).

According to the second law of thermodynamics (*entropy criterion*) specialized to isothermal motions, the energy release rate on a discontinuity is non-negative:

$$D\left[\int_{u_+}^{u_-} \sigma\, du - \frac{\sigma_+ + \sigma_-}{2}(u_+ - u_-)\right] \geqq 0\,. \tag{2.16}$$

Other restrictions follow if we expect physically realizable discontinuous solutions to arise as limits of solutions of some appropriately regularized set of equations. Thus, according to the *viscosity criterion* the jump discontinuity is admissible if the states on both sides may be connected by a travelling wave of the system (2.2) which is regularized by including a viscosity term proportional to the strain rate in the stress constitutive equation:

$$\sigma = \sigma(u) + \eta u_t, \tag{2.17}$$

where η is the effective viscosity coefficient. Discontinuities admissible by the viscosity criterion automatically satisfy (2.16). They include waves that comply with the *chord* (*Oleinik*) *condition*:

$$\begin{aligned} &\text{if } D > 0, \text{ then } \frac{\sigma(u) - \sigma(u_+)}{u - u_+} \leqq \frac{\sigma(u_-) - \sigma(u_+)}{u_- - u_+} \text{ for all } u_+ \leqq u \leqq u_-, \\ &\text{if } D < 0, \text{ then } \frac{\sigma(u) - \sigma(u_+)}{u - u_+} \leqq \frac{\sigma(u_-) - \sigma(u_+)}{u_- - u_+} \text{ for all } u_+ \geqq u \geqq u_-, \end{aligned} \tag{2.18}$$

plus all nontrivial stationary waves with $D = 0$ (cf. SLEMROD (1983), PEGO (1987)).

Another principle for selection, employed by LAX (1971) in full generality for genuinely nonlinear systems, is the requirement of stability of weak solutions. According to the Lax admissibility criterion characteristics of one family from both sides meet on the discontinuity, while the characteristics of the other families cross through the discontinuity. For system (2.2) this means that admissible waves are supersonic with respect to the state ahead and subsonic with respect to the state behind. With our constitutive assumptions (2.4), the system (2.2) is not genuinely nonlinear and characteristics must be permitted to become tangent to the discontinuity. Therefore, following ISAACSON et al. (1990) we introduce a *generalized Lax criterion* which allows for states for which either

$$c(u_+) \leqq \sqrt{\frac{\sigma(u_+) - \sigma(u_-)}{u_+ - u_-}} \leqq c(u_-)$$

or

$$c(u_+) \geqq \sqrt{\frac{\sigma(u_+) - \sigma(u_-)}{u_+ - u_-}} \geqq c(u_-), \tag{2.19}$$

depending on whether $D \gtrless 0$. For the forward-moving discontinuities with $D > 0$, this condition, long known in gas dynamics, means that the shock is supersonic or sonic with respect to a state ahead and subsonic or sonic with respect to a state behind.

If $\sigma(u)$ is strictly convex or concave, all three of the criteria ((2.16), (2.18) and (2.19)) prove to be equivalent. For the material with $\sigma(u)$ depicted as in Fig. 1, they impose different restrictions on u_+ and u_-; the corresponding admissible areas in the (u_+, u_-) plane are schematically shown on Fig. 2 for the forward moving jump discontinuities. (For the rest of the paper without loss of generality we assume that $D \geqq 0$.)

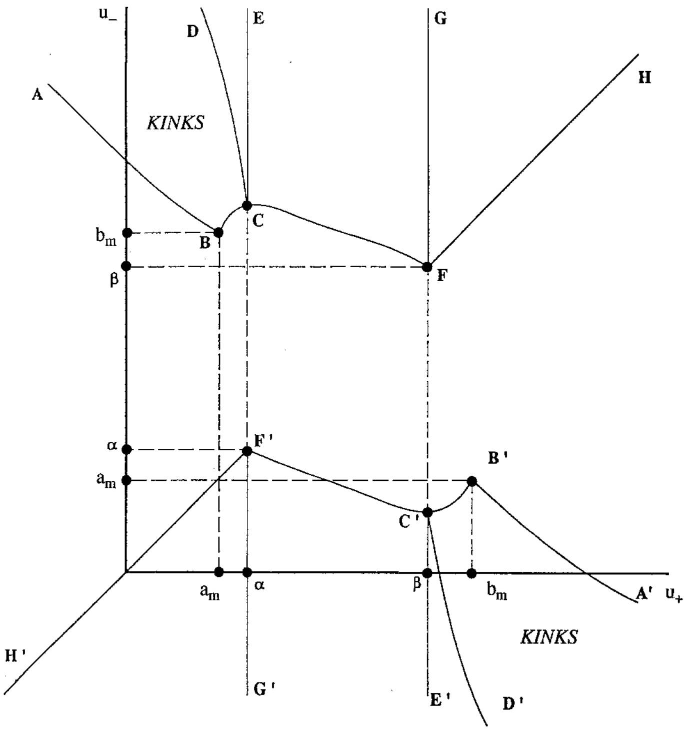

Fig. 2. Restrictions imposed by different admissibility conditions on the values of u_+ and u_- adjacent to the jump discontinuity with $D \geqq 0$. Domains *GFH* and *G'F'H'* correspond to classical shock waves, *ECD* and *E'C'D'* to supersonic phase boundaries, *ABCD* and *A'B'C'D'* to subsonic phase boundaries (kinks). The generalized Lax criterion (2.19) is satisfied in both *GFH* (*G'F'H'*) and *ECD* (*E'C'D'*), while the chord condition (2.18) is satisfied everywhere in the domain *DCFH* (*D'C'F'H'*).

We now define the boundaries of the areas indicated in Fig. 2:
1. *FH* and *F'H'* (degenerate shocks)

$$u_{+} = u_{-}, \tag{2.20}$$

2. *AB* and *A'B'* (Maxwell or dissipation-free regimes)

$$\int_{u_-}^{u_+} \sigma \, du = \frac{\sigma(u_+) + \sigma(u_-)}{2} (u_+ - u_-), \tag{2.21}$$

3. *CD* and *C'D'* (Chapman-Jouguet or sonic regimes)

$$\sigma(u_-) - \sigma(u_+) = c^2(u_+)(u_- - u_+), \tag{2.22}$$

4. *BCF* and *B'C'F'* (stationary shocks)

$$\sigma(u_+) = \sigma(u_-). \tag{2.23}$$

By construction, the curve *AB* is described by the function $u_- = b_2(u_+)$, the curve *CD* is represented by the function $u_- = b_3(u_+)$ the segment *BC* corresponds to $u_- = b_1(u_+)$, whereas *CF* is its obvious continuation into the elliptic domain $u_+ > \alpha$. For the sake of simplicity, we assume that the state behind the discontinuity u_- is always in the β-phase. In this way we restrict our discussion to the domain *ABCFH* (recall that $D \geqq 0$ throughout the paper).

The condition (2.16) forbids points (u_+, u_-) outside domain *ABCFH* (and *A'B'C'F'H'*). All three admissibility criteria mentioned above are satisfied for the discontinuities having values (u_+, u_-) in the domains *GFH* (classical shock waves) and *DCE* (sonic and supersonic phase boundaries). We use the collective term *conventional shocks* for solutions (u_+, u_-, v_+, v_-) of (2.13) with (u_+, u_-) in these domains. Discontinuities in the domain *ECFG*, representing transformations of the states in the elliptic region $u_+ \in (\alpha, \beta)$, are not considered here.

One can see that the points (u_+, u_-) from the open domain (see domain *ABCD* on Fig. 2)

$$\begin{aligned} a_m \leqq u_+ \leqq \alpha, \quad & b_1(u_+) \leqq u_- < b_3(u_+), \\ u_+ \leqq a_m, \quad & b_2(u_+) \leqq u_- < b_3(u_+), \end{aligned} \tag{2.24}$$

correspond to kinks which are subsonic with respect to the state ahead. All kinks in the domain (2.24) are admissible according to the entropy criterion (2.16). The viscosity criterion allows only particular kinks, namely, those on the line *CB* (see Fig. 2). This is an example of a selection criterion which may depend on the type of the regularization. The necessity of an extra jump condition of the form $f(u_+, u_-, D) = 0$ for subsonic kinks, often called a *kinetic relation*, is discussed from different perspectives in ABEYARATNE & KNOWLES (1987, 1990, 1991 a), GURTIN & STRUTHERS (1990) and TRUSKINOVSKY (1982, 1987, 1993 a). For the rest of the paper we adopt the following *admissibility criterion*:

1. All conventional shocks are admissible, (*)
2. Admissible kinks are selected by a prescribed kinetic relation of the form

$$f(u_+, u_-, D) = 0,$$

having the property that all solutions (u_+, u_-, D) *of* $f(u_+, u_-, D) = 0$ *satisfy the entropy criterion* (2.16).

For the subsequent analysis a specific form of the kinetic relation will not be important.

3. Formulation of the problem

Consider a kink described by a piecewise constant solution of the system (2.2)

$$(u, v)(x, t) = \begin{cases} (a, 0), & x \geqq Dt, \\ (b, v_b), & x < Dt, \end{cases} \tag{3.1}$$

where the pair $(u_+ = a,\ u_- = b)$ is in the domain $ABCD$ of Fig. 2. In (3.1) we denote by v_b the particle velocity of the state behind the discontinuity, and we have applied Galilean invariance to put $v(x, t) = 0$, $x > Dt$, without loss of generality. The velocity $D \geqq 0$ of our kink is related to a and b by

$$D(a, b) = \sqrt{\frac{\sigma(b) - \sigma(a)}{b - a}}, \tag{3.2}$$

while

$$v_b = -\sqrt{(\sigma(b) - \sigma(a))(b - a)} \tag{3.3}$$

in accordance with (2.15) and the assumption that $D \geqq 0$. The particular choice of the state behind the kink is restricted by a kinetic relation whose particular form is irrelevant at the moment.

Consider the solution (3.1) at an arbitrary instant of time $t = t_0$ as providing piecewise constant initial data for the system (2.2). By changing variables $(x, t) \to (x, t - t_0)$ we can take $t_0 = 0$. Then at $t = 0$, we have special initial data

$$(u, v)(x, 0) = \begin{cases} (a, 0), & x \geqq 0, \\ (b, v_b), & x < 0, \end{cases} \tag{3.4}$$

where a, b and v_b are related through (3.2), (3.3) and the kinetic relation $f(a, b, D(a, b)) = 0$. The question arises as to whether the continuation (3.1) is unique, or whether the states $(a, 0)$ and (b, v_b) may be connected by *another system of waves*. A straightforward search through the self-similar combinations of fans, shocks and kinks, compatible with the initial data (3.4), suggests the following as a candidate (see a similar analysis in PENCE (1992)):

$$(u,v)(\xi)=\begin{cases}(a,0), & c(a)\,t<x<\infty,\\ (u(\xi),v(\xi)), & c(q)\,t<x<c(a)\,t,\\ (s,v_s), & -D_s t<x<c(q)\,t,\\ (b,v_b), & -\infty<x<-D_s t.\end{cases} \tag{3.5}$$

Here $\xi=x/t$, $u(\xi)$ is implicitly given by $c(u)=\xi$,

$$v(\xi)=-\int_a^{u(\xi)} c(\mu)\,d\mu,$$

and the parameters s, q, D_s, v_s and v_b with $s \geqq b_1(a)$, $q \leqq \alpha$ are related by

$$c(q)=\sqrt{\frac{\sigma(s)-\sigma(q)}{s-q}}, \tag{3.6}$$

$$v_s=-\int_a^q c(u)\,du-\sqrt{(\sigma(s)-\sigma(q))(s-q)}, \tag{3.7}$$

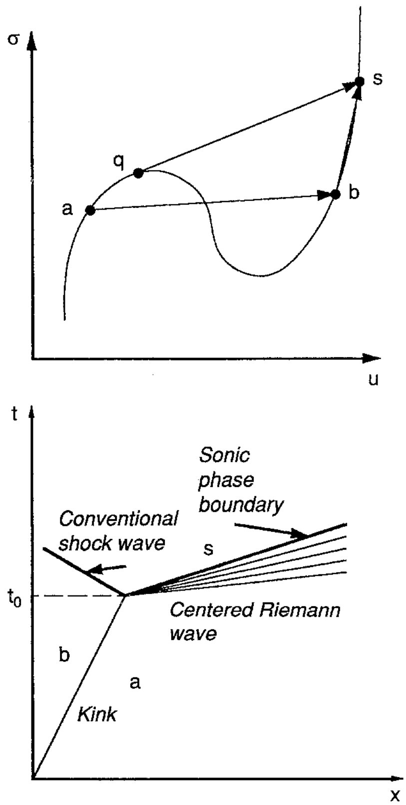

Fig. 3. A schematic illustration of the break-up of a steadily propagating subsonic phase boundary (kink $a \to b$); $a \to q$ is a centered Riemann wave, $b \to s$ is a classical shock wave, and $q \to s$ is a sonic phase boundary.

$$D_s = \sqrt{\frac{\sigma(s) - \sigma(b)}{s - b}}, \tag{3.8}$$

$$v_s = v_b + \sqrt{(\sigma(s) - \sigma(b))(s - b)}\,. \tag{3.9}$$

If (3.5)–(3.9) has a solution, its geometric meaning is clear from Fig. 3. A forward moving Riemann wave (fan) $a \to q$, where q is implicitly given by (3.6), travels with a local characteristic speed $c(a)$. In the wave the strain smoothly grows from a to q, while the velocity changes from 0 to $-\int_a^q c(u)\,du$. The fan is followed by an attached sonic phase boundary which also travels to the right in Fig. 3 with the local sonic speed $c(q) \leqq c(a)$. The strain jumps abruptly inside this wave from q (α-phase) to s (β-phase). The velocity behind the phase boundary v_s is given by (3.7). At the same time a classical shock wave moves to the left with the supersonic speed $D_s \geqq c(b)$, which satisfies (3.8). The particle velocity behind the shock is provided by (3.9).

The two formulae (3.7) and (3.9) must give the same expression for v_s, which is possible if and only if the nonlinear equation

$$-\sqrt{(\sigma(b) - \sigma(a))(b - a)} + \sqrt{(\sigma(s) - \sigma(b))(s - b)}$$
$$= -\int_a^q c(u)\,du - \sqrt{(\sigma(s) - \sigma(q))(s - q)}\,, \tag{3.10}$$

where q and s are implicitly related by (3.6), has a solution. In equation (3.10) the pair (a, b) represents a given point in the domain of kinks $ABCD$ (see Fig. 2). In the next section we characterize the subdomain of $ABCD$, where equation (3.10) has a unique solution $s = s(a, b)$.

4. The main theorem

In Section 3 the original problem was reformulated as an algebraic one. Here we give a complete solution of this algebraic problem.

Suppose $q(s) \leqq \alpha$ is the solution of the equation $b_3(q) = s$. We define for $(a, b) \in ABCD$ and $s \geqq b_* \overset{\text{def}}{=} b_1(\alpha)$ two auxiliary functions

$$P(a, s) = \int_a^{q(s)} c(u)\,du + \sqrt{(\sigma(s) - \sigma(q(s)))(s - q(s))}\,, \tag{4.1}$$

$$Q(a, b, s) = D(a, b)(b - a) - D(s, b)(s - b)\,. \tag{4.2}$$

Also, we define for $a \leqq \alpha$ the set

$$b_4(a) = \{b > b_m : \tilde{P}(a) = \tilde{Q}(a, b)\}, \tag{4.3}$$

where

$$\tilde{P}(a) = P(a, b_*)\,, \tag{4.4}$$

$$\tilde{Q}(a, b) = Q(a, b, b_*) \tag{4.5}$$

are restrictions of P and Q to the line $s = b_*$. According to Section 3, to prove the existence of a nontrivial solution of our Riemann problem (3.5) it is sufficient to find, for a given pair (a, b) from $ABCD$, a function $s(a, b) \geqq b_*$ such that

$$Q(a, b, s) = P(a, s). \tag{4.6}$$

Our main results will be that $b_4(a) \neq \emptyset$ and that equation (4.6) has a unique solution $s(a, b)$ for $b > \min\{\inf b_4(a),\ b_2(a)\}$ and $a \leqq \alpha$.

We begin with a characterization of the location of the subset $b = b_4(a)$ inside the domain $ABCD$. According to (2.24), for the stress-strain relation, shown at Fig. 1, $(a, b) \in ABCD$ if

$$\begin{aligned} a_m \leqq a \leqq \alpha \quad &\text{and } b_1(a) \leqq b < b_3(a), \quad \text{or if} \\ a \leqq a_m \quad &\text{and } b_2(a) \leqq b < b_3(a). \end{aligned} \tag{4.7}$$

This follows from the monotonicity of $b_1(a)$, $b_2(a)$ and $b_3(a)$:

$$\frac{db_1}{da} = \frac{c^2(a)}{c^2(b_1(a))} \geqq 0, \tag{4.8}$$

$$\frac{db_2}{da} = \frac{c^2(a) - D^2(b_2(a), a)}{D^2(b_2(a), a) - c^2(b_2(a))} < 0, \tag{4.9}$$

$$\frac{db_3}{da} = \frac{\sigma''(a)}{c^2(b_3(a)) - D^2(b_3(a), a)} < 0, \tag{4.10}$$

and the inequalities (see Fig. 4)

$$b_3(a) > b_2(a), \quad b_3(a) \geqq b_1(a)$$

(also note that $b_2(a_m) = b_1(a_m)$, $b_1(\alpha) = b_3(\alpha)$).

Let $a = \tilde{\tilde{a}} < a_m$ be a solution of $b_2(a) = b_*\,(\equiv b_1(\alpha))$. The location of the set $b = b_4(a)$ for a belonging to a subinterval of $(\tilde{\tilde{a}}, \alpha)$ is provided by

Lemma. *There exists a unique* $\tilde{a} \in (\tilde{\tilde{a}}, a_m)$ *such that for all* $a \in [\tilde{a}, \alpha]$ *the equation*

$$\tilde{P}(a) = \tilde{Q}(a, b) \tag{4.11}$$

has a unique solution $b = b_4(a)$. *Moreover, if* $a \in [a_m, \alpha]$, *then* $b_4(a) \in [b_1(a), b_*]$; *if* $a \in [\tilde{a}, a_m]$, *then* $b_4(a) \in [b_2(a), b_*]$ *and* $b_4(\tilde{a}) = b_2(\tilde{a})$.

Proof. The proof is based on a careful ordering of $\tilde{P}$ and $\tilde{Q}$ on the boundaries of the domain $\tilde{\tilde{A}}CB$, where the point $\tilde{\tilde{A}}$ has coordinates $(\tilde{\tilde{a}}, b_2(\tilde{\tilde{a}}))$ (see Fig. 4). We first show that

$$\tilde{P}(a) \leqq \tilde{Q}(a, b_*). \tag{4.12}$$

In fact, according to the Schwarz inequality,

$$\int_a^\alpha c(u)\, du \leqq \sqrt{(\sigma(\alpha) - \sigma(a))(\alpha - a)}\,;$$

therefore

$$\tilde{P}(a) \leqq D(\alpha, a)(\alpha - a)\,. \tag{4.13}$$

On the other hand, since $b_* > \alpha$, the comparison of the areas of the two enclosed rectangles on the (σ, u)-plane with diagonals $(\sigma(a), a) - (\sigma(\alpha), \alpha)$ and $(\sigma(a), a) - (\sigma(b_*), b_*)$ gives

$$\tilde{Q}(a, b_*) = \sqrt{(\sigma(b_*) - \sigma(a))(b_* - a)} \geqq D(\alpha, a)(\alpha - a)\,.$$

Combined with (4.13), this inequality proves (4.12). One can see that (4.12) is in fact strict unless $a = \alpha$. Now, by definition,

$$Q(a, b_1(a)) = -D(b_*, b_1(a))(b_* - b_1(a)) \leqq 0\,,$$

while $\tilde{P}(a) \geqq 0$, whence

$$\tilde{P}(a) \geqq \tilde{Q}(a, b_1(a))\,, \tag{4.14}$$

and the inequality is again strict unless $a = \alpha$.

Consider further restrictions of the functions $\tilde{P}$ and $\tilde{Q}$ on the line $b = b_2(a)$ (the line $B\tilde{A}\tilde{\tilde{A}}A$ on Fig. 4). Introduce

$$\tilde{\tilde{P}}(a) = \tilde{P}(a)\,, \quad \tilde{\tilde{Q}}(a) = \tilde{Q}(a, b_2(a))\,.$$

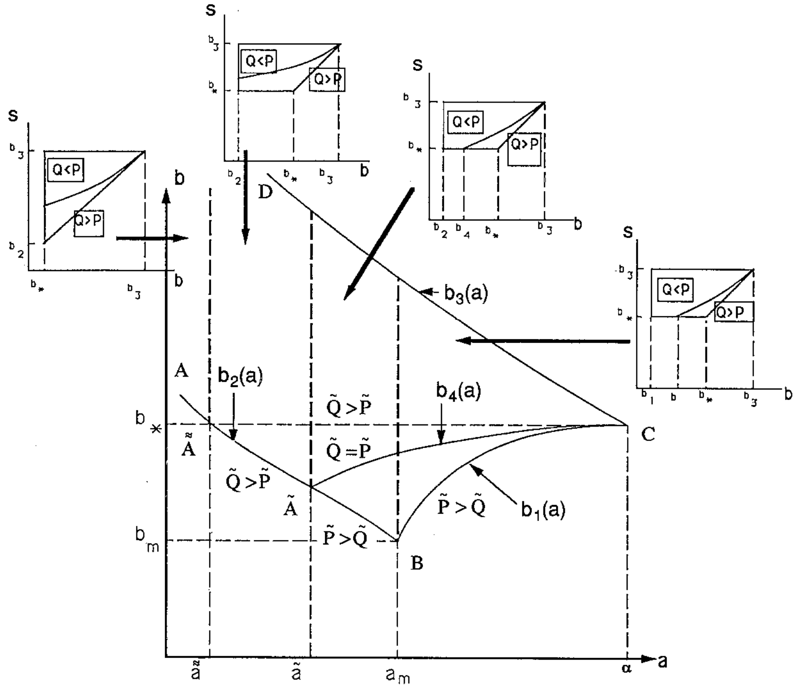

Fig. 4. Schematic illustration of the proof of the lemma and the main theorem. Shown are the domain $ABCD$ of kinks and the triangular domain $\tilde{A}BC$ outside of which the nontrivial solution (3.5) exists.

By the same reasoning that we used to get (4.12) and (4.14), we establish that at the point $B = (a_m, b_m)$ (see Fig. 4)

$$\tilde{\tilde{P}}(a_m) > \tilde{\tilde{Q}}(a_m),$$

while at the point $\tilde{A} = (\tilde{a}, b_2(\tilde{a}))$ (on Fig. 4)

$$\tilde{\tilde{P}}(\tilde{\tilde{a}}) < \tilde{\tilde{Q}}(\tilde{\tilde{a}}).$$

We conclude that on $B\tilde{A}\tilde{\tilde{A}}$ there exists at least one point where $\tilde{\tilde{P}} = \tilde{\tilde{Q}}$, which we denote by $\tilde{a}$. This point is unique, since both $\tilde{\tilde{P}}$ and $\tilde{\tilde{Q}}$ are strictly monotone. In fact, one can show that

$$\frac{d\tilde{\tilde{P}}}{da} \equiv \frac{d\tilde{P}}{da} = -c(a) < 0, \qquad \frac{d\tilde{\tilde{Q}}}{da} \equiv \frac{\partial\tilde{Q}}{\partial a} + \frac{\partial\tilde{Q}}{\partial b}\frac{db_2}{da} < 0$$

for $a \leqq \alpha$. The last inequality can be checked by a direct calculation:

$$\begin{aligned} \frac{\partial\tilde{Q}}{\partial a} &= -\frac{1}{2}\frac{c^2(a) + D^2(a, b)}{D(a, b)} < 0, \\ \frac{\partial\tilde{Q}}{\partial b} &= \frac{1}{2}\left[\frac{c^2(b) + D^2(a, b)}{D(a, b)} + \frac{c^2(b) + D^2(a, b_*)}{D(a, b_*)}\right] > 0. \end{aligned} \tag{4.15}$$

We also recall from (4.9) that $db_2/da < 0$.

The rest of the proof is immediate from the established ordering of $\tilde{P}$ and $\tilde{Q}$ on the three lines $b = b_*(\tilde{A}C)$, $b = b_1(a)(BC)$ and $b = b_2(a)(B\tilde{\tilde{A}})$, the monotonicity of $\tilde{Q}$ as a function of b, established by (4.15), and the inequality

$$\frac{db_4}{da} = \frac{\dfrac{\frac{1}{2}(c^2(b) + D^2(a, b)) - c(b)D(a, b)}{D(a, b)}}{\dfrac{1}{2}\left[\dfrac{c^2(b) + D^2(a, b)}{D(a, b)} + \dfrac{c^2(b) + D^2(a, b_*)}{D(a, b_*)}\right]} \geqq 0. \qquad \square$$

Now we are in a position to formulate the main theorem.

Theorem. *Suppose that* $a \in [\tilde{\tilde{a}}, \alpha]$ *and* $b \in [b_4(a), b_3(a))$ *or that* $a < \tilde{\tilde{a}}$ *and* $b \in [b_2(a), b_3(a))$. *Then the nonlinear equation* (4.6) *has a unique solution* $s = s(a, b)$.

Proof. The proof of the Theorem is based on ideas similar to those used to prove the Lemma. We first show that

$$Q(a, b, b_3(a)) \leqq P(a, b_3(a)). \tag{4.16}$$

Since the expression $(\sigma(b)-\sigma(a))(b-a)$ represents an area of a rectangle with a diagonal $(a,\sigma(a))$, $(b,\sigma(b))$ and since $b_3(a)\geqq b$ and $\sigma(b_3)\geqq\sigma(b)$, it is obvious that

$$\sqrt{(\sigma(b_3(a))-\sigma(a))(b_3(a)-a)}\geqq\sqrt{(\sigma(b)-\sigma(a))(b-a)}\,. \tag{4.17}$$

Now, by definition,

$$Q(a,b,b_3(a))=\sqrt{(\sigma(b)-\sigma(a))(b-a)}-\sqrt{(\sigma(b_3(a))-\sigma(b))(b_3(a)-b)}\,,$$

$$P(a,b_3(a))=\sqrt{(\sigma(b_3(a))-\sigma(a))(b_3(a)-a))}\,,$$

so inequality (4.17) implies (4.16). By the same reasoning, (4.16) is strict unless $b=b_3(a)$.

The next step is to establish the sign of the difference $Q-P$ along the line $s=b$. First we note that

$$Q(a,b_3(a),b_3(a))=P(a,b_3(a)) \tag{4.18}$$

while from the Lemma (see (4.12))

$$Q(a,b_*,b_*)>P(a,b_*) \tag{4.19}$$

if $a<\alpha$. Next we calculate derivatives of Q and P along the line $s=b\,(b\geqq b_*)$ at given a, to obtain

$$\frac{d}{db}Q(a,b,b)=\frac{1}{2}\frac{c^2(b)+D^2(a,b)}{D(a,b)}\geqq 0, \tag{4.20}$$

$$\frac{d}{db}P(a,b)=\frac{1}{2}\frac{c^2(b)+c^2(q(b))}{c(q(b))}\geqq 0. \tag{4.21}$$

From (4.18), (4.19) and inequalities (4.20), (4.21) we conclude that

$$Q(a,b,b)\geqq P(a,b) \tag{4.22}$$

and the inequality is strict except when $a=\alpha$ or $b=b_3$. Now, as one can see from Fig. 4, the existence part of the Theorem follows immediately from (4.16), (4.22), and the Lemma.

To prove uniqueness it is sufficient to establish suitable monotonicity properties of the functions $-Q$ and P with respect to s. A straightforward calculation provides the desired result:

$$\frac{\partial Q(a,b,s)}{\partial s}=-\frac{1}{2}\frac{c^2(s)+D^2(s,b)}{D(s,b)}\leqq 0,$$

$$\frac{\partial P(a,s)}{\partial s}=\frac{1}{2}\frac{c^2(s)+c^2(q(s))}{c(q(s))}>0$$

for $(a,b)\in A\tilde{A}CD$ and $s\in\{\max\{b_2(a),b_*,b_3(a)\}$ (see Fig. 4). These inequalities, together with the information on the relative values of P and Q on the boundary of the admissible region (see Fig. 4), ensure the existence of a unique $s=s(a,b)$ which satisfies (4.6) everywhere except in the triangular domain $\tilde{A}BC$. □

Remark. R. JAMES pointed out to me that the inequality (4.22) has a purely geometrical nature. In fact, by the Schwarz inequality (see the proof of the Lemma)

$$P(a, s) - Q(a, b, s) \leqq D(a, q(s))(q(s) - a) + D(s, q(s))(s - q(s))$$
$$- D(a, b)(b - a) + D(s, b)(s - b).$$

In particular,

$$P(a, b) - Q(a, b, b) \leqq D(a, q(b))(q(b) - a) + D(s, q(b))(b - q(b))$$
$$- D(a, b)(b - a).$$

But $\sqrt{\mu\nu} + \sqrt{\eta\xi} \leqq \sqrt{(\mu + \nu)(\eta + \xi)}$ and therefore

$$D(a, q(b))(q(b) - a) + D(q(b), b)(b - q(b)) - D(a, b)(b - a) \leqq 0,$$

which proves (4.22).

5. Entropy-rate criterion

It seems appropriate to attempt to single out physically admissible solutions by employing the *entropy-rate admissibility criterion*, suggested by DAFERMOS (1973). DAFERMOS' criterion states that the rate of entropy growth, which is equivalent in our isothermal setting to the rate of release of mechanical energy, is not smaller for the *admissible* solution than for any other solution of the same initial-value problem. This criterion has been successfully used to narrow the class of solutions in both hyperbolic and mixed-type problems (cf. HATTORI (1986), PENCE (1992), ABEYARATNE & KNOWLES (1992)).

The energy dissipation in isothermal, conservative elastodynamics takes place at jump discontinuities. For the Riemann problem the formula for the rate of decay of the total mechanical energy was given by DAFERMOS (1973):

$$R = \sum_i D(u_-, u_+) A(u_-, u_+), \tag{5.1}$$

where

$$A(u_-, u_+) = \int_{u_-}^{u_+} \sigma(u)\, du - \frac{\sigma(u_+) + \sigma(u_-)}{2}(u_+ - u_-), \tag{5.2}$$

and summation is carried out over all discontinuities.

Let us apply this criterion to our initial-value problem (3.4). For the trivial solution (3.1),

$$R_t(a, b) = D(a, b)\left[\int_b^a \sigma(u)\, du - \frac{\sigma(a) + \sigma(b)}{2}(a - b)\right],$$

while for the split solution (3.5),

$$R_s(a, b) = D(s, q)\left[\int_s^q \sigma\, du - \frac{\sigma(s) + \sigma(q)}{2}(q - s)\right]$$

$$- D(s, b)\left[\int_b^s \sigma\, du - \frac{\sigma(s) + \sigma(b)}{2}(s - b)\right]$$

where $q = q(s)$ is a solution of (3.6), and $s(a, b)$ is a solution of (3.10), defined for $(a, b) \in A\tilde{A}CD$. It follows from the definition that both solutions are identical at $b = b_3(a)$, so that

$$R_t(a, b_3(a)) = R_s(a, b_3(a)). \tag{5.3}$$

Direct calculation of $R_t(a, b)$ and $R_s(a, b)$ for the cubic $\sigma(u)$ (equation (2.8)) shows that for sufficiently fast phase boundaries $(b \leqq b_3(a))$, the rate of entropy production is larger for the split solution than for the single-wave solution, while slow enough kinks dissipate energy faster than the alternative multiwave solution.

Hence in this case there exists $b = b_5(a)$ such that

$$R_t(a, b) \geqq R_s(a, b) \quad \text{if } \max\{b_2(a), b_4(a)\} \leqq b \leqq b_5(a),$$

$$R_t(a, b) \leqq R_s(a, b) \quad \text{if } b_5(a) \leqq b \leqq b_3(a).$$

The graph of $b = b_5(a)$ calculated for the cubic $\sigma(u)$ as in (2.8) with

$$a_m = 0, \quad b_m = 1, \quad k = 1, \quad \sigma_m = 0 \tag{5.4}$$

is shown on Fig. 5.

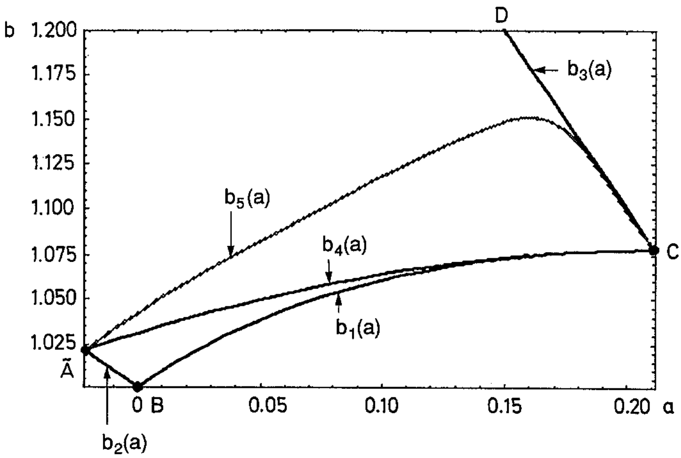

Fig. 5. The domain of existence and the Dafermos limit for the "split" solution obtained numerically for the material with the cubic stress-strain relation (2.8) with parameters (5.4).

According to Dafermos' criterion for $b \geqq b_5(a)$ the trivial solution (3.1) cannot be admissible. We note that this is an interesting case for the nontrivial solution when the existence boundary $b = b_4(a)$ and the admissibility boundary $b = b_5(a)$ do not coincide.

6. Viscosity-capillarity model

The above mode of instability *is not operating* if we consider as admissible only those kinks and conventional shocks that are selected by the *viscosity-capillarity criterion* (TRUSKINOVSKY (1982), SLEMROD (1983), SHEARER (1983), ABEYARATNE & KNOWLES (1991 b)). This criterion is based on the availability of a continuous description for the kink as a travelling-wave solution of the regularized system of equations.

In the viscosity-capillarity model, the constitutive equation for stress (2.17) is augmented by the introduction of a strain-gradient term:

$$\sigma = \sigma(u) + \eta v_x - 2\varepsilon u_{xx} \tag{6.1}$$

where $\varepsilon > 0$ is a parameter of the *conservative* part of the constitutive model; this brings an internal scale of length into the theory. To derive the corresponding restrictions on u_+ and u_-, we substitute the ansatz $u(\zeta)$, $v(\zeta)$, where $\zeta = x - Dt$, into (2.2), (6.1) and integrate once to get a boundary-value problem for a second-order ordinary differential equation:

$$\sigma(u) - D^2 u - \eta D \dot{u} - 2\varepsilon \ddot{u} = \sigma(u_+) - D^2 u_+ , \tag{6.2}$$

$$u(\pm\infty) = u_\pm , \qquad \dot{u}(\pm\infty) = 0 , \tag{6.3}$$

where the superposed dot denotes the ζ derivative. One can show (see TRUSKINOVSKY (1993 a, 1993 b)) that if the pair (u_+, u_-) is in the domain of kinks *ABCD*, the boundary-value problem (6.2), (6.3) has no solution unless u_+ and u_- satisfy a certain relation of the type $f(u_+, u_-, D) = 0$ supplementary to the ordinary Rankine-Hugoniot conditions. This is a particular kinetic relation. If the boundary values u_+ and u_- are anywhere inside the domain of classical shocks *GFH*, the solution of (6.2) exists unconditionally. If, however, the pair (u_+, u_-) is in the domain of the supersonic and sonic phase boundaries *DCE*, the corresponding discontinuity may or may not be admissible by the viscosity-capillarity criterion, depending on the value of the nondimensional ratio $W = \eta/\sqrt{\varepsilon}$.

For example, consider the special case when $\sigma(u)$ is a cubic polynomial as given by the expression (2.8). Thus if (u_+, u_-) is in *ABCD* (kink), then the boundary-value problem (6.2), (6.3) has a solution if and only if u_+ and u_- are related by the following kinetic relation (TRUSKINOVSKY (1987, 1993 b)):

$$3\left(1 - \frac{12}{W^2}\right)\left(\frac{u_+ + u_-}{b_m - a_m} - \frac{b_m + a_m}{b_m - a_m}\right)^2 + \left(\frac{u_- - u_+}{b_m - a_m}\right)^2 = 1 . \tag{6.4}$$

For the sonic or supersonic shock ($u_+ = a$, $u_- = b$) in the domain DCE one can show that the boundary-value problem (6.2), (6.3) has a solution if and only if $b \geqq \phi(a)$. The function $\phi(a)$ is defined by the condition that the pair $(u_+, u_-) = \big(1.5(a_m + b_m) - \phi(a) - a,\ \phi(a)\big)$ satisfies (6.4). This follows from the fact that if $(u_+, u_-) \in DCE$, then for the dynamical system (6.2) (with $\sigma(u)$ from (2.8)) the unstable manifold of the saddle at $(u, \dot{u}) = (u_-, 0)$ either is attracted by the stable node (focus) at $(u, \dot{u}) = (u_+, 0)$, which happens when the shock is admissible by the viscosity-capillarity criterion, or goes to infinity, which happens when the shock is not admissible; the borderline case when there exist a heteroclinic trajectory connecting the saddle at $(u, \dot{u}) = (u_-, 0)$ with another saddle at $(u, \dot{u}) = \big(1.5(a_m + b_m) - u_- - u_+, 0\big)$ is provided by the condition (6.4) above (see also SHEARER & YANG (1992)). The domain of admissible discontinuities is shown in Fig. 6 for $W = 4$.

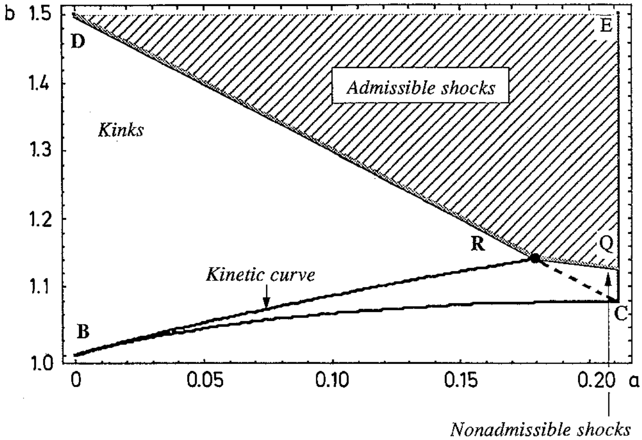

Fig. 6. Jump discontinuities admissible by the viscosity-capillarity criterion for the cubic $\sigma(u)$ from (2.8) with parameters (5.4) and $W = 4$. Points B, C, D, E have the same meaning as in Figs. 2, 4. The kinetic curve BR is obtained from (6.4). The curve RQ is a solution of $b = \phi(a)$.

As we see, in contrast to the purely viscous case ($W = \infty$), the general viscosity-capillarity criterion imposes restrictions on some of the conventional shocks. Therefore the supersonic waves admissible by our criterion (*) are not necessarily admissible by the viscosity-capillarity criterion. Moreover, one can show that the sonic phase boundaries which are not admissible by the viscosity-capillarity criterion are those required for the split solution to exist. This also follows from the uniqueness theorems for the Riemann problem of FAN & SLEMROD (1991), SHEARER & YANG (1992). That the class of conventional shocks admissible by the viscosity-capillarity criterion is *much narrower* than the class of shocks admissible by the generalized Lax criterion may be viewed as an indication of an inadequacy of the regularization scheme (6.1).

7. Discussion

In the previous sections we saw that two weak solutions of a system of nonlinear conservation laws (2.2) could have the same initial data if the admissibility criterion (*) from Section 2 is adopted. Since the initial configuration ought to determine the state of deformation in the future, only one of these solutions should occur in nature and the other ought to be excluded on the basis of some additional *physical* principle, which is not contained in our simplified equations. The clarification of the cause of the nonuniqueness is also important for computations since numerical algorithms are usually deterministic and always lead to a definite result.

In order to pick out the physically meaningful solution, it is important to decide in what sense the established nonuniqueness corresponds to instability. For example, one can view the "nonuniqueness" as implying that the initial data in fact *differ* for the two solutions. The only place where these data can deviate is at point $x = 0$.

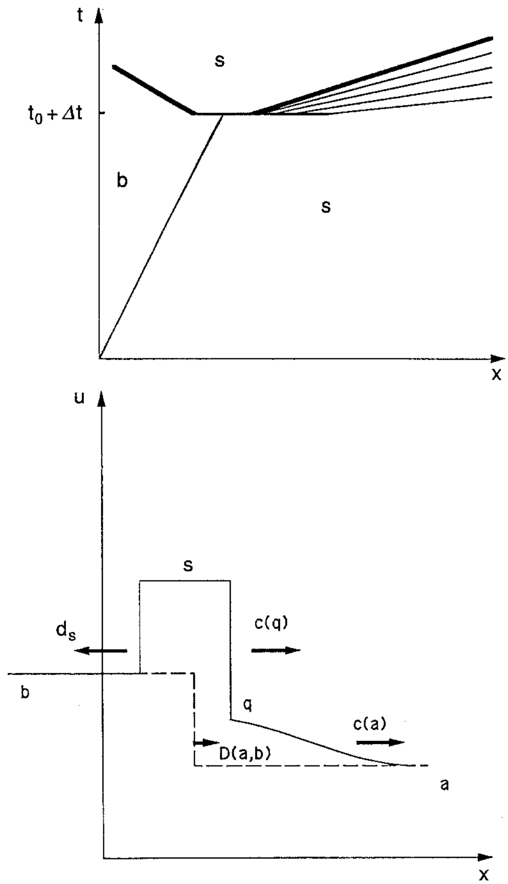

Fig. 7. Schematic illustration of the finite perturbation (7.1), which is responsible for the instability.

To fix the ideas, consider an alternative solution (3.5) at $t = \Delta t$:

$$(u, v)(x, t) = \begin{cases} (a, 0), & c(a)\,\Delta t < x < \infty, \\ (u(\zeta), v(\zeta)), & c(q)\,\Delta t < x < c(a)\,\Delta t, \\ (s, v_s), & -D_s\,\Delta t < x < c(q)\,\Delta t, \\ (b, v_b), & -\infty < x < -D_s\,\Delta t, \end{cases} \tag{7.1}$$

where all notations are as in (3.5). One can view (7.1) as a new set of initial data at $t = 0$ and consider it as a perturbation of (3.4) localized at the segment $[-D_s\,\Delta t, c(a)\,\Delta t]$ (see Fig. 7). In the limit $\Delta t \to 0$, the support of the perturbation (7.1) (parametrized by Δt) tends to the point $t = 0$, which proves the local instability of the trivial solution, at least in L^1. The perturbation (7.1), however, does not converge pointwise to zero as $\Delta t \to 0$. Of course, the usual definition of weak solution for hyperbolic conservation laws does not make the distinction we are trying to clarify, so we are really advocating a different approach that accounts directly for nucleation events (cf. ABEYARATNE & KNOWLES (1991 a)). In the regularized theory the existence of an internal scale of length (or time) does not allow the limit $\Delta t \to 0$, and the critical nucleus analogous to (7.1) cannot be considered a "small" perturbation, even in L^1. In this sense the single-wave solutions is metastable rather than unstable. Physically, the system requires an adequate perturbation (nucleation event) to overcome the energy barrier, which depends on this internal scale. One can speculate that the availability of this perturbation is related to the presence of highly localized constitutive or geometrical imperfections.

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Department of Aerospace Engineering and Mechanics
University of Minnesota
Minneapolis, Minnesota 55455

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