MATERIAL INSTABILITIES AND THE CALCULUS OF VARIATIONS

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1. INTRODUCTION.

The aim of the calculus of variations is to study the minimization of integrals depending on unknown functions. In continuum mechanics a common procedure is to minimize a 'free energy' integral, the minimizing functions being interpreted as equilibrium displacement and temperature fields. The motivation lies in thermodynamics. Roughly, we seek an appropriate Lyapunov function for the governing equations, typically of the form

$$E(u) = \int_{\text{body}} \mathscr{F}(X, J^k u(X,t))\,dX,$$

where u is a vector of field variables (displacement, velocity, density, temperature etc.) and $J^k u$ denotes the set of all partial derivatives of u with respect to X of all orders r with $0 \leqslant r \leqslant k$; that is, $E(u(\cdot,t))$ is a non-increasing function of time t along solutions. Often we add the extra requirement that $E(u(\cdot,t))$ is constant if and only if $u = u(X)$ is a time-independent solution. In general there may be many time-independent solutions, infinitely many in the case of some problems involving phase transitions, leading to complicated behaviour of solutions as $t \longrightarrow \infty$. Some solutions may have atypical asymptotic behaviour, converging, for example, to unstable time-independent solutions. However, in the presence of a Lyapunov function E we expect that such exceptional solutions will lie in a negligible

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subset N of the phase space X of admissible functions. We further expect that the remainder $X\setminus N$ of the phase space is the disjoint union of 'larger' positively invariant sets S_α and that solution paths u in S_α are minimizing for E, i.e.

$$\lim_{t\to\infty} E(u(\cdot,t)) = \inf_{v\in S_\alpha} E(v).$$

In particular, if $t_j \longrightarrow \infty$ then $v_j(x) = u(x,t_j)$ will be a <u>minimizing sequence</u> for E in S_α, i.e.

$$E(v_j) \searrow \inf_{v\in S_\alpha} E(v).$$

In especially favourable cases there may be just one $S_\alpha = X$ with N empty and all solution paths minimizing for E in X. In general a particular S_α might contain a number of time-independent solutions with the same value of E, or no time-independent solution at all.

For specific problems the following natural questions are important:

(Q1) Do the governing equations admit one or more nontrivial Lyapunov function E ?

(Q2) Given an appropriate subset S of X, does E attain a minimum on S ?

(Q3) What conditions does a minimizer satisfy?

(Q4) Do all minimizing sequences for E on S tend to minimizers? If not, what happens?

(Q5) When <u>is</u> $u(\cdot,t_j)$ a minimizing sequence, and what special properties do such sequences, realized by the dynamics, possess?

(Q6) What can be said about the structure of the decomposition $X = N \cup \bigcup_\alpha S_\alpha$?

These questions are particularly interesting for materials which can undergo phase transitions; typically the governing equations can then change type (cf Ericksen [20]). In this article we make some remarks concerning the first four questions but say nothing about the last two, about which little is known. (Some partial, but inconclusive, information about (Q5) was obtained in a model problem by Andrews & Ball [2].)

2. LYAPUNOV FUNCTIONS IN NONLINEAR THERMOELASTICITY.

We address (Q1) - (Q3) in the context of a nonlinear thermoelastic material. The results are taken from joint work with G. Knowles [6] that is still in progress. Some of the calculations are formal, and no attempt is made to make precise all the hypotheses concerning regularity etc.

We are concerned with a thermoelastic material occupying the bounded strongly Lipschitz open subset $\Omega \subset \mathbb{R}^n$ in a reference configuration. At time t the particle occupying the point $X \in \Omega$ in the reference configuration has position $x(X,t) \in \mathbb{R}^n$ and temperature $\theta(X,t) > 0$. For simplicity we suppose that there is no external body force or heat supply. The governing equations are then

$$\rho_R \ddot{x} = \mathrm{Div}\, T_R, \tag{2.1}$$

$$\rho_R \dot{U} - \mathrm{tr}(T_R \dot{F}^T) + \mathrm{Div}\, q_R = 0, \tag{2.2}$$

where $\rho_R(X)$ is the density in the reference configuration, T_R is the Piola-Kirchhoff stress tensor, U is the internal energy density, $F = \nabla x(X,t)$ is the deformation gradient, and q_R is the (reference) heat flux vector. The constitutive relations are given in terms of the Helmholtz free energy $A(X,F,\theta)$ and specific entropy $\eta(X,F,\theta)$ by

$$\left.\begin{aligned} & T_R = \rho_R \frac{\partial A}{\partial F}, \quad \eta = -\frac{\partial A}{\partial \theta}, \quad U = A + \eta\theta, \\ & q_R = q_R(X,F,\theta,\mathrm{Grad}\,\theta). \end{aligned}\right\} \tag{2.3}$$

The second law of thermodynamics requires that

$$q_R \cdot \mathrm{Grad}\,\theta \leqslant 0, \tag{2.4}$$

and we shall assume that this inequality is strict for $\mathrm{Grad}\,\theta \neq 0$.

We impose the following boundary conditions:

$$\underline{\text{Mechanical}} \qquad \left.\begin{aligned} & x = x_0(X) \quad \text{on } \partial\Omega_1, \\ & T_R N = 0 \quad \text{on } \partial\Omega \setminus \partial\Omega_1. \end{aligned}\right\} \tag{2.5}$$

$$\underline{\text{Thermal}} \qquad \left.\begin{aligned} & \theta = \theta_0(X) \quad \text{on } \partial\Omega_2, \\ & q_R \cdot N = 0 \quad \text{on } \partial\Omega \setminus \partial\Omega_2. \end{aligned}\right\} \tag{2.6}$$

Here $\partial\Omega_1$, $\partial\Omega_2$ are given subsets of the boundary $\partial\Omega$, $N = N(X)$ is the unit outward normal to $\partial\Omega$ at X, and $x_o, \theta_o > 0$ are given functions.

We define $\mathscr{F} = \mathscr{F}(X, \dot{x}, F, \theta)$ by

$$\mathscr{F} = \rho_R\left[\frac{1}{2}|\dot{x}|^2 + U - \phi(X)\eta\right],$$

where $\phi(X)$ is specified later.

A standard computation using (2.1) - (2.3) and (2.5) yields

$$\frac{d}{dt}\int_\Omega \mathscr{F} dX = \int_\Omega \left(\frac{\phi}{\theta} - 1\right) \operatorname{Div} q_R \, dX$$

$$= \int_{\partial\Omega}\left(\frac{\phi}{\theta} - 1\right) q_R \cdot N dA - \int_\Omega \left(\frac{\phi}{\theta}\right)_{,\alpha} q_R^\alpha dX. \tag{2.7}$$

Provided that $\phi\Big|_{\partial\Omega_2} = \theta_o\Big|_{\partial\Omega_2}$ the surface integral vanishes by (2.6).

<u>Special cases</u>

1. Suppose θ_o is independent of X. In this case we choose $\phi \equiv \theta_o$ and (2.7) becomes, using (2.4),

$$\frac{d}{dt}\int_\Omega \mathscr{F} dX = \theta_o \int_\Omega \frac{q_R \cdot \operatorname{Grad}\theta}{\theta^2} dX \leq 0.$$

The result is well known; cf Duhem [16], Ericksen [18], Coleman & Dill [11], for example. The function $\mathscr{F} = \rho_R\left[\frac{1}{2}|\dot{x}|^2 + U - \theta_o\eta\right]$ is known as the <u>equilibrium free energy</u>.

2. Suppose that $q_R = q_R(X, \theta, \operatorname{Grad}\theta)$, and let ϕ satisfy the stationary heat equation

$$\operatorname{Div} q_R(X, \phi, \operatorname{Grad}\phi) = 0 \quad \text{in } \Omega \tag{2.8}$$

with the same boundary conditions as θ, namely

$$\left.\begin{aligned} \phi &= \theta_o(X) && \text{on } \partial\Omega_2, \\ q_R(X, \phi, \operatorname{Grad}\phi)\cdot N &= 0 && \text{on } \partial\Omega\setminus\partial\Omega_2. \end{aligned}\right\} \tag{2.9}$$

(In the examples considered below ϕ is unique.) By (2.7),

$\int_\Omega \mathscr{F} dX$ is a Lyapunov function provided

$$I(\theta) \stackrel{\text{def}}{=} \int_\Omega \left(\frac{\phi}{\theta}\right)_{,\alpha} q_R^\alpha(X,\theta,\text{Grad}\,\theta)\,dX \geqslant 0$$

for all $\theta > 0$ satisfying (2.6). It is easily verified that $\theta = \phi$ is a solution of the Euler-Lagrange equations for I. Since $I(\phi) = 0$ we are faced with a classical question in the calculus of variations, to decide if the given solution ϕ is a global minimum of I. The problem is not trivial because ϕ is only known implicitly and because the integrand may be negative. One interesting case which can be handled is when $q_R = -k(\theta)\text{Grad}\,\theta$, with the thermal conductivity $k(\theta)$ assumed positive. In this case $I(\theta) \geqslant 0$ if $\frac{\theta k'(\theta)}{k(\theta)}$ is a nonincreasing function of θ; conversely, if $\frac{\theta k'(\theta)}{k(\theta)}$ is non-decreasing and not constant then there exist domains Ω and boundary conditions (2.6) for which I may be negative. For the proofs and further results see [6]. To illustrate one of the methods for analyzing I consider the anisotropic linear case

$$q_R = -K(X)\,\text{Grad}\,\theta\,,$$

where the matrix $K(X)$ is positive for each X. Then letting $w = \log\theta - \log\phi$ we obtain

$$\begin{aligned} I(\theta) &= \int_\Omega -\left(\frac{\phi}{\theta}\right)_{,\alpha} K^{\alpha\beta}\theta_{,\beta}\,dX \\ &= \int_\Omega \left[\phi K^{\alpha\beta}w_{,\alpha}w_{,\beta} + K^{\alpha\beta}\phi_{,\beta}w_{,\alpha}\right]dX \\ &\geqslant \int_\Omega K^{\alpha\beta}\phi_{,\beta}w_{,\alpha}\,dX = \int_\Omega \left[(K^{\alpha\beta}\phi_{,\beta}w)_{,\alpha} - w(K^{\alpha\beta}\phi_{,\beta})_{,\alpha}\right]dX \\ &= \int_{\partial\Omega} K^{\alpha\beta}\phi_{,\beta}wN_\alpha\,dA = 0. \end{aligned}$$

In particular, setting $T_R = 0$, $U = \theta$ we see that

$$\frac{d}{dt}\int_\Omega \rho_R(\theta - \phi\log\theta)\,dX \leqslant 0 \tag{2.10}$$

for positive solutions θ, satisfying (2.6), of the linear heat equation

$$\rho_R \frac{\partial\theta}{\partial t} = \mathrm{Div}(K(X)\,\mathrm{Grad}\,\theta). \tag{2.11}$$

If $(x(\cdot),v(\cdot),\theta(\cdot))$ is a local minimum of

$$E(x,v,\theta) \stackrel{\mathrm{def}}{=} \int_\Omega \rho_R\left[\frac{1}{2}|v|^2 + U(X,\nabla x,\theta) - \phi(X)\eta(X,\nabla x,\theta)\right]dX$$

subject to the boundary conditions (2.5),(2.6) then formally we have that

$$v = 0, \tag{2.12}$$

$$\rho_R\left(\frac{\partial U}{\partial\theta} - \phi\,\frac{\partial\eta}{\partial\theta}\right) = 0, \tag{2.13}$$

and

$$\mathrm{Div}\,\rho_R\left(\frac{\partial U}{\partial F} - \phi\,\frac{\partial\eta}{\partial F}\right) = 0. \tag{2.14}$$

Using the thermodynamic identities (2.3) we obtain from (2.13) that

$$(\theta-\phi)\frac{\partial\eta}{\partial\theta} = 0,$$

which, assuming that the specific heat $\frac{\partial\eta}{\partial\theta}$ is positive, yields

$$\theta = \phi. \tag{2.15}$$

(This is what motivates the choice of ϕ in the special cases above.)

From (2.3),(2.14) and (2.15) we obtain

$$\mathrm{Div}\,T_R = 0, \tag{2.16}$$

the usual equilibrium equation.

Special care has to be taken in the case when $\partial\Omega_2$ is empty, since then

$$\frac{d}{dt}\int_\Omega \rho_R\left(\frac{1}{2}|\dot{x}|^2 + U\right)dX = 0$$

for solutions of (2.1),(2.2),(2.5),(2.6), so that setting $v = \dot{x}$ we have

$$\int_\Omega \rho_R\left(\frac{1}{2}|v|^2 + U\right)dX = E_0, \tag{2.17}$$

where E_0 is a constant given by the initial data. Taking $\phi = 1$, it follows that $-\int_\Omega \rho_R \eta\, dX$ is a Lyapunov function. A local minimum of $-\int_\Omega \rho_R\eta\,dX$ subject to (2.17) and the boundary conditions (2.5),(2.6) formally satisfies

$$\rho_R\left(\frac{\partial\eta}{\partial\theta} - \lambda\,\frac{\partial U}{\partial\theta}\right) = 0\ , \tag{2.18}$$

$$\lambda\rho_R v = 0\ , \tag{2.19}$$

and

$$\mathrm{Div}\ \rho_R\left(\frac{\partial\eta}{\partial F} - \lambda\,\frac{\partial U}{\partial F}\right) = 0\ , \tag{2.20}$$

where λ is a Lagrange multiplier. If $\frac{\partial\eta}{\partial\theta} > 0$ then (cf Ericksen [18]) we deduce from (2.18) that

$$\theta = \frac{1}{\lambda} = \text{constant}\ ,$$

and thus $v = 0$ and (2.16) again holds. Similar considerations apply whenever the governing equations of a system possess conserved quantities (e.g. the mass constraint (3.8) below), and reinforce the need for a complete knowledge of all such conserved quantities.

Given appropriate existence theorems for minimizers (see [3,9]) it is not altogether obvious how to establish rigorously necessary conditions such as (2.16); some information on this question is given in [5].

3. MINIMIZERS AND MINIMIZING SEQUENCES FOR INVISCID FLUIDS WITH HEAT CONDUCTION.

In this section we consider (Q1) - (Q3), and especially (Q4), for an inviscid fluid with heat conduction. The results are taken from joint work with G. Knowles [6] that is still in progress and to which the reader is referred for a more detailed description. The fluid is assumed to be homogeneous and to occupy the spatial region $\omega \subset \mathbb{R}^n$, where ω is bounded and open. At time t and position $x \in \omega$ the fluid has density $\rho(x,t) \geqslant 0$, velocity $v(x,t) \in \mathbb{R}^n$ and temperature $\theta(x,t) > 0$. For simplicity we assume that there is no external body force or heat supply. The governing equations are then

$$\rho\dot{v} = -\ \mathrm{grad}\, p\ , \tag{3.1}$$

$$\dot{\rho} + \rho\,\mathrm{div}\, v = 0\ , \tag{3.2}$$

$$\rho\dot{U} + p\,\mathrm{div}\, v + \mathrm{div}\, q = 0\ , \tag{3.3}$$

where dots denote material time derivatives, p is the pressure, U is the internal energy density and q is the (spatial) heat flux vector. The constitutive relations are given in terms of the Helmholtz free energy $A(\rho,\theta)$ and specific entropy $\eta(\rho,\theta)$ by

$$\left.\begin{array}{l} p = \rho^2 \dfrac{\partial A}{\partial \rho}, \ \eta = -\dfrac{\partial A}{\partial \theta}, \ U = A + \eta\theta, \\ q = q(\rho,\theta,\operatorname{grad}\theta). \end{array}\right\} \tag{3.4}$$

The second law of thermodynamics requires that

$$q\cdot\operatorname{grad}\theta \leqslant 0, \tag{3.5}$$

and we assume that this inequality is strict for $\operatorname{grad}\theta \neq 0$. We impose the boundary conditions

$$\left.\begin{array}{l} v\cdot n\Big|_{\partial\omega} = 0, \\ \theta\Big|_{\partial\omega_2} = \theta_0, \quad q\cdot n\Big|_{\partial\omega\setminus\partial\omega_2} = 0 \end{array}\right\} \tag{3.6}$$

where $\partial\omega_2$ is a nonempty subset of the boundary $\partial\omega$, $n = n(x)$ is the unit outward normal to $\partial\omega$ at x, and $\theta_0 > 0$ is constant.

As in the previous section, solutions of (3.1) - (3.6) satisfy

$$\frac{d}{dt}\int_\omega \rho\left(\frac{1}{2}|v|^2 + U - \theta_0\eta\right)dx = \theta_0 \int_\omega \frac{q\cdot\operatorname{grad}\theta}{\theta^2}\,dx \leqslant 0 \tag{3.7}$$

(cf [11]). We also have the mass constraint

$$\int_\omega \rho\,dx = M, \tag{3.8}$$

where the constant $M > 0$ is determined by the initial data.

Corresponding to (3.7) our aim is to study the absolute minimizers and minimizing sequences of

$$E(\rho,v,\theta) \stackrel{\text{def}}{=} \int_\omega \rho\left(\frac{1}{2}|v|^2 + U(\rho,\theta) - \theta_0\eta(\rho,\theta)\right)dx \tag{3.9}$$

subject to the constraint (3.8). We make the following hypotheses on $A(\rho,\theta)$:

(i) $A : (0,b)\times(0,\infty) \longrightarrow \mathbb{R}$ is continuous, where $b > 0$ is a constant,

(ii) for each fixed $\rho \in (0,b)$, $A(\rho,\cdot)$ is C^1 and strictly concave,

(iii) for each fixed $\theta \in (0,\infty)$, the function $f_\theta(\rho) \overset{\text{def}}{=} \rho A(\rho,\theta)$ satisfies $\lim_{\rho\to 0+} f_\theta(\rho) = 0$,
$$\lim_{\rho\to 0+} \frac{f_\theta(\rho)}{\rho} = -\infty \quad\text{and}\quad \lim_{\rho\to b-} f_\theta(\rho) = +\infty.$$

These hypotheses are satisfied by the classical van der Waals' fluid (cf Landau & Lifshitz [23]) for which

$$A(\rho,\theta) = -a\rho + k\theta\log\left(\frac{\rho}{b-\rho}\right) - c\theta\log\theta - d\theta + \text{const.}, \tag{3.10}$$

where the coefficients a, k and c are positive.

By (ii)

$$A(\rho,\theta) \leqslant A(\rho,\theta_o) + (\theta-\theta_o)\frac{\partial A}{\partial\theta}(\rho,\theta_o),$$

with equality if and only if $\theta = \theta_o$. Thus the integrand in (3.9) has a strict minimum, for fixed ρ, when $v = 0$ and $\theta = \theta_o$. Motivated by this, we consider the problem of minimizing

$$I(\rho) \overset{\text{def}}{=} \int_\omega \rho(U(\rho,\theta_o) - \theta_o\eta(\rho,\theta_o))dx$$
$$= \int_\omega f_{\theta_o}(\rho(x))dx$$

among measurable functions $\rho : \omega \longrightarrow [0,b]$ satisfying (3.8), where $f_{\theta_o}(b)$ is defined to be $+\infty$ in consonance with (iii).

We are interested in cases, such as (3.10), for which $f_{\theta_o}(\cdot)$ is not convex. We denote by $f^{**}_{\theta_o}$ the <u>lower convex envelope</u> of f_{θ_o}, that is

$$f^{**}_{\theta_o}(\rho) = \sup\{\alpha + \beta\rho : \alpha + \beta t \leqslant f_{\theta_o}(t) \text{ for all } t \in [0,b)\},$$

and by $\mathcal{W}$ the <u>Weierstrass set</u>

$$\mathcal{W} = \{\rho \in [0,b) : f^{**}_{\theta_o}(\rho) = f_{\theta_o}(\rho)\}.$$

Recall that if $F : [0,b) \longrightarrow \mathbb{R}$ then the subdifferential $\partial F(\rho)$ of F at the point $\rho \in [0,b)$ is defined to be the set

$$\partial F(\rho) \overset{\text{def}}{=} \{\beta \in \mathbb{R} : F(\rho) + \beta(t-\rho) \leqslant F(t) \text{ for all } t \in [0,b)\}.$$

Define

$$S(\bar\rho) = \{\rho \in (0,b) : \partial f^{**}_{\theta_o}(\bar\rho) \subset \partial f_{\theta_o}(\rho)\},$$

where $\bar{\rho} = \frac{M}{\text{meas}\,\omega}$ is the mean density. It is easily shown that $S(\bar{\rho}) \subset \mathcal{W}$ and, using (iii), that $\bar{\rho}$ belongs to the convex hull of $S(\bar{\rho})$. In the case of (3.10), for $\frac{ab}{k\theta_o} > \left(\frac{3}{2}\right)^3$ there exists exactly one nontrivial common tangent to the graph of f_{θ_o} with end-points ρ_1, ρ_2 as shown in Figure 1. The Weierstrass set $\mathcal{W} = [0,\rho_1] \cup [\rho_2, b)$, and $S(\bar{\rho}) = \{\bar{\rho}\}$ for $\bar{\rho} \in (0,\rho_1) \cup (\rho_2, b)$, $S(\bar{\rho}) = \{\rho_1\} \cup \{\rho_2\}$ for $\bar{\rho} \in [\rho_1, \rho_2]$. In order to characterize the minimizing

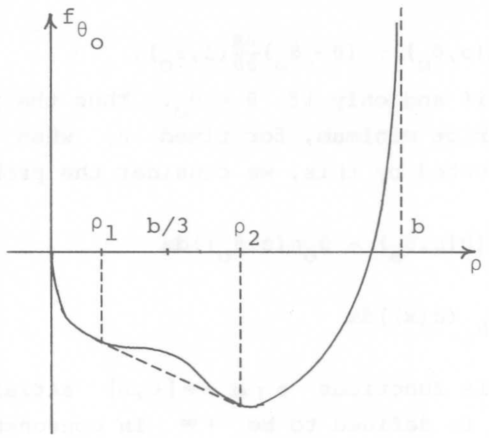

Figure 1

The graph of f_{θ_o} *for a van der Waals' fluid*

sequences of I we introduce, following L.C. Young [30] (see also McShane [24], Berliocchi & Lasry [10], Tartar [27]), the generalized problem:

Minimize

$$\hat{I}(\nu) \stackrel{\text{def}}{=} \int_\omega \int_{[0,b]} f_{\theta_o}(\rho)\, d\nu_x(\rho)\, dx$$

subject to

$$\int_\omega \int_{[0,b]} \rho\, d\nu_x(\rho)\, dx = M. \qquad (3.11)$$

The unknown $\nu = (\nu_x)$ is a Young measure, that is a measurable mapping $x \mapsto \nu_x$ of ω to probability measures on $[0,b]$. (Due to the results of Tartar [27,28] and DiPerna

[14,15] these measures are playing an increasing rôle in the study of nonlinear partial differential equations. Their use in the calculus of variations is now standard; see, for example, the article by Jean Taylor in this volume.) An ordinary function $\rho(x)$ corresponds to the Young measure $\nu_x = \delta_{\rho(x)}$; note that for this ν we have $\hat{I}(\nu) = I(\rho)$ and $\int_\omega \int_{[0,b]} \rho d\nu_x(\rho)dx = \int_\omega \rho(x)dx$.

Theorem 3.1

(a) *The minimum of* $\hat{I}(\nu)$ *subject to (3.11) is attained; the minimizing Young measures* $\bar{\nu}$ *are exactly those satisfying (3.11) and such that* $\operatorname{supp}\bar{\nu}_x \subset S(\bar{\rho})$ *a.e.* $x \in \omega$.

(b) *The minimum value of* I *subject to (3.8) is the same as that of* $\hat{I}(\nu)$ *subject to (3.11), and is attained exactly by those functions* ρ *satisfying (3.8) and such that* $\rho(x) \in S(\bar{\rho})$ *a.e.* $x \in \omega$.

(c) *Let* $\{\rho_j\}$ *be any minimizing sequence for* I *subject to (3.8); then there exists a subsequence* $\{\rho_\mu\}$ *and a minimizing Young measure* $\bar{\nu}$ *for* $\hat{I}$ *subject to (3.11), such that for any continuous function* $F:[0,b] \longrightarrow \mathbb{R}$,

$$F(\rho_\mu) \xrightarrow{*} \int_{[0,b]} F(\rho)d\bar{\nu}_x(\rho) \quad \textit{in} \quad L^\infty(\omega). \tag{3.12}$$

Conversely, given any minimizing Young measure $\bar{\nu}$ *for* $\hat{I}$ *subject to (3.11) there exists a minimizing sequence* $\{\rho_\mu\}$ *of* I *subject to (3.8) satisfying (3.12).*

Part (b) of the theorem is a result of a type first stated by Gibbs [21]; a similar, but not identical version is given by Dunn & Fosdick [17 Theorem 9].

The proof of Theorem 3.1 is given in [6], where a variety of similar problems are also considered. Here we merely note that part (a) follows by integration of the inequality

$$f(\rho) \geqslant f(\tilde{\rho}) + \beta(\rho - \tilde{\rho}), \ \rho \in [0,b], \ \tilde{\rho} \in S(\bar{\rho}), \ \beta \in \partial f_{\theta_0}^{**}(\bar{\rho}),$$

with respect to $\bar{\nu}_x, \nu_x$ and ω.

Applying part (a) to $f_{\theta_o}^{**}$, and noting that $\partial f_{\theta_o}^{**}(\rho) = \partial f_{\theta_o}(\rho)$ for any $\rho \in \mathcal{W}$, we see that the minimizing Young measures $\bar{\nu}$ of $\hat{I}$ are the same as those of

$$\hat{I}^{**}(\nu) = \int_\omega \int_{[0,b]} f_{\theta_o}^{**}(\rho)\,d\nu_x(\rho)\,dx,$$

and hence that the infimum of I is unchanged if f_{θ_o} is replaced by $f_{\theta_o}^{**}$. It follows using lower semicontinuity that any minimizing sequence of I has a subsequence converging weak $*$ in $L^\infty(\omega)$ to a minimizer of

$$I^{**}(\rho) = \int_\omega f_{\theta_o}^{**}(\rho(x))\,dx$$

subject to (3.8). A result closely related to this was proved by Dacorogna [12] in material coordinates. The appearance of the lower convex envelope of f_{θ_o} is consistent with results of statistical physics for infinite volumes (for discussion and references see Thompson [29]); these results establish convexity properties of certain averaged free energy functions, but do not appear to give information concerning the local free energy A. Note that part (b) of the theorem shows that only values of $\rho \in \mathcal{W}$ can be observed in an absolute minimizer; this is the classical <u>Weierstrass condition</u> of the calculus of variations. Sometimes it is erroneously asserted that because of this 'stability' condition f_{θ_o} is itself convex; the correct interpretation noted above has been pointed out by, for example, Ericksen [18].

Using Theorem 3.1 it can be shown that any minimizing sequence (ρ_j, v_j, θ_j) of E subject to (3.8) possesses a subsequence $(\rho_\mu, v_\mu, \theta_\mu)$ such that $v_\mu \longrightarrow 0$ a.e., $\theta_\mu \longrightarrow \theta_o$ a.e., and ρ_μ converges to a minimizer $\bar{\nu}$ of $\hat{I}$ in the sense of (3.12). Similarly, the minimizers of E have the form $(\rho, 0, \theta_o)$, where ρ is a minimizer of I. It follows from part (c) of the theorem that in general (e.g. for the van der Waals' fluid) there are minimizing sequences (ρ_j, v_j, θ_j) with ρ_j converging in the sense of (3.12) to a Young measure $\bar{\nu}$ which does not correspond to a function, and such that $\rho_j \xrightarrow{*} \rho$ in $L^\infty(\omega)$ with ρ <u>not</u> a minimizer of I. Typically these sequences 'mix the phases' more and more finely as j increases. It would be very interesting to know if such sequences can be realized by the dynamics (cf (Q5) and Andrews & Ball [2]). Such dynamic behaviour would be physically significant in regimes where the phases are mixed sufficiently coarsely to neglect the energy of phase boundaries.

Finally we note that by part (b) of the theorem, any minimizer $(\rho, 0, \theta_0)$ of E satisfies

$$f_{\theta_0}'(\rho(x)) = \text{const.}\ , \quad f_{\theta_0}(\rho(x)) - \rho(x) f_{\theta_0}'(\rho(x)) = \text{const.}\ ,$$

a.e. in ω, provided $A(\rho,\theta)$ is C^1 in ρ. These are the familiar necessary conditions representing constancy of the chemical potential and pressure respectively.

4. QUASICONVEXITY AND ELASTIC STABILITY

We consider a nonlinear thermoelastic material as in §2. For simplicity we suppose that the material is homogeneous, so that ρ_R and A do not depend explicitly on X. In contrast to §2 we suppose that there is a conservative body force $\rho_R b = \nabla_x \Psi(X,x)$, so that (2.1) now becomes

$$\rho_R \ddot{x} = \operatorname{Div} T_R + \rho_R b. \tag{4.1}$$

We assume that the boundary conditions are as in §2, special case 1, with $\partial\Omega_2$ nonempty. The same calculation as usual shows that if

$$\mathscr{F} = \rho_R\left[\frac{1}{2}|\dot{x}|^2 + U - \theta_0\eta\right] + \Psi$$

then $\frac{d}{dt}\int_\Omega \mathscr{F} dX \leqslant 0$. Assuming that A is strictly concave in θ and applying the reasoning in §3, we are led to consider the problem of minimizing

$$I(x) = \int_\Omega [W(\nabla x(X)) + \Psi(X,x(X))]\,dX \tag{4.2}$$

subject to (2.5), where the stored-energy function W is defined by

$$W(F) \stackrel{\text{def}}{=} \rho_R A(F,\theta_0). \tag{4.3}$$

We suppose that $W : M^{n\times n} \longrightarrow \overline{\mathbb{R}}$ is continuous (with respect to the usual topology of the extended real line $\overline{\mathbb{R}}$) and bounded below, where $M^{n\times n}$ denotes the set of all real $n \times n$ matrices, and that $\Psi : \overline{\Omega} \times \mathbb{R}^n \longrightarrow \mathbb{R}$ is continuous and bounded below.

The following definition is an adaptation of that of Morrey [26].

Definition ([9])

Let $1 \leqslant p \leqslant \infty$. W is $W^{1,p}$-quasiconvex at $A \in M^{n\times n}$ if

$$\int_D W(A + \nabla\phi(Y))dY \geqslant \int_D W(A)dY$$

for every bounded open set $D \subset \mathbb{R}^n$ with meas $\partial D = 0$ and all ϕ belonging to the Sobolev space $W_0^{1,p}(D;\mathbb{R}^n)$. If this holds for all $A \in M^{n\times n}$ we say that W is $W^{1,p}$-quasiconvex.

We attempt to illuminate this somewhat impenetrable condition by stating some recent results.

Theorem 4.1 (Ball & Murat [9])

Let $A \in M^{n\times n}$, *and suppose that* $I(x)$ *attains a minimum on* $AX + W_0^{1,p}(\Omega;\mathbb{R}^n)$ *for every smooth nonnegative* Ψ. *Then* W *is* $W^{1,p}$-*quasiconvex at* A.

It is possible that I is sequentially weakly lower semicontinuous on $W^{1,p}(\Omega;\mathbb{R}^n)$ (weak $*$ if $p = \infty$) if and only if W is $W^{1,p}$-quasiconvex but so far only partial results have been obtained (see [9] for the references). Relaxation theorems of the type given in §3 expressed in terms of lower quasiconvex envelopes (but not making use of the Young measure) have been given by Acerbi & Fusco [1] and Dacorogna [13], though these have not as yet been shown to hold under weak enough growth conditions to apply to elasticity.

Definitions

(a) By a standard boundary region with normal $N \in \mathbb{R}^n$ we mean a bounded strongly Lipschitz domain $D \subset \mathbb{R}^n$ satisfying

(i) D is contained in the half-space $K_a^N = \{X \in \mathbb{R}^n : X\cdot N < a\}$ for some $a \in \mathbb{R}^n$, and

(ii) the $n-1$ dimensional interior E of $\partial D \cap K_a^N$ is nonempty; we denote $\partial D \setminus E$ by ∂D_1.

(b) Let $x \in W^{1,1}(\Omega;\mathbb{R}^n)$ be such that $I(x)$ exists and is finite, and let $X_o \in \overline{\Omega}$. We say that x is a <u>local minimum of</u> I <u>at</u> X_o <u>in</u> $W^{r,p} \cap C^o$ if there are numbers $\rho > 0$, $\delta > 0$ such that $I(y)$ exists and $I(y) \geqslant I(x)$ whenever $y - x \in C^\infty(\overline{\Omega};\mathbb{R}^n)$, $y(X) = x(X)$ for $|X - X_o| > \rho$ and $X \in \overline{\Omega}$, and $\|y - x\|_{W^{r,p}(\Omega;\mathbb{R}^n)} + \|y - x\|_{C^o(\overline{\Omega};\mathbb{R}^n)} < \delta$.

<u>Theorem 4.2</u> (a special case of Ball & Marsden [7 Thm 2.2])

Let $1 \leqslant p < \infty$ *and let* r *be a positive integer satisfying* $r < 1 + \frac{n}{p}$. *Suppose* $x \in W^{1,1}(\Omega;\mathbb{R}^n)$ *is a local minimum of* I *at* $X_o \in \overline{\Omega}$ *in* $W^{r,p} \cap C^o$ *and that* x *is* C^1 *in a neighbourhood of* X_o *in* $\overline{\Omega}$.

(i) If $X_o \in \Omega$, *then*

$$\int_D W(\nabla x(X_o) + \nabla\phi(Y))\,dY \geqslant \int_D W(\nabla x(X_o))\,dY$$

for any bounded open set $D \subset \mathbb{R}^n$ *and all* $\phi \in C_o^1(D;\mathbb{R}^n)$ *(=* C^1 *functions with compact support in* D*) satisfying* $\det(\nabla x(X_o) + \nabla\phi(Y)) > 0$ *for all* $Y \in \overline{D}$.

(ii) Let $X_o \in \partial\Omega \setminus \partial\overline{\Omega}_1$, *and suppose* $\partial\Omega$ *is smooth in a neighbourhood of* X_o. *Let* $N = N(X_o)$ *be the unit outward normal to* $\partial\Omega$ *at* X_o, *and let* D *be a standard boundary region with normal* N. *Then*

$$\int_D W(\nabla x(X_o) + \nabla\phi(Y))\,dY \geqslant \int_D W(\nabla x(X_o))\,dY$$

for all $\phi \in C^1(\overline{D};\mathbb{R}^n)$ *vanishing in a neighbourhood of* ∂D_1 *in* $\overline{D}$ *and such that* $\det(\nabla x(X_o) + \nabla\phi(Y)) > 0$ *in* $\overline{D}$.

Part (i) of the theorem is but a slight generalization of a result of Meyers [25 pp128-131]; note that the conclusion is nearly that W is $W^{1,\infty}$-quasiconvex at $\nabla x(X_o)$. The condition in part (ii) of the theorem is a <u>quasiconvexity condition at the boundary</u>; roughly, it asserts that $z(Y) = \nabla x(X_o)Y$ minimizes $\int_D W(\nabla z(Y))\,dY$ <u>globally</u> subject to the boundary condition $z|_{\partial D_1} = \nabla x(X_o)Y|_{\partial D_1}$. In [7] part

(ii) is used for $n > 1$ to construct an example of a strictly quasiconvex, strictly polyconvex W having a natural state that is not a local minimum of $J(x) \overset{\text{def}}{=} \int_\Omega W(\nabla x)\,dX$ in $W^{r,p} \cap C^0$ for $r < 1 + \frac{n}{p}$ even though the second variation of J is strictly positive (linearized stability); this cannot happen for $n = 1$. The technical hypotheses in results such as Theorem 4.2 could do with some improvement to allow less regularity of $x(\cdot)$ and $\phi(\cdot)$.

Example (cf [4,9])

Let $n = 3$ and define

$$W(F) = \operatorname{tr}(F^T F) + h(\det F), \tag{4.4}$$

where h is convex, $h(\delta) = +\infty$ for $\delta \leqslant 0$, h is continuous for $\delta > 0$, and $\lim_{\delta \to 0+} h(\delta) = \lim_{\delta \to \infty} \frac{h(\delta)}{\delta} = \infty$. Then W is $W^{1,p}$-quasiconvex if and only if $p \geqslant 3$. In fact if $1 \leqslant p < 3$ then W is not $W^{1,p}$-quasiconvex at $\lambda 1$ for $\lambda > 0$ sufficiently large; this corresponds to the fact that a solid ball B made of this material and subjected to the radial boundary displacement $x(X)\big|_{\partial B} = \lambda X$ can reduce its energy by cavitation, i.e. by forming a hole in its interior. The stored-energy function (4.4) is of a type used to model natural rubber, which can rupture by cavitation.

Given a stored-energy function $W(F)$ one may define for $1 \leqslant p \leqslant \infty$ the sets

$$S_p = \{F : W \text{ is } W^{1,p}\text{-quasiconvex at } F\}.$$

Clearly $S_p \subset S_q$ if $p \leqslant q$. Anticipating the proof of refinements of Theorem 4.2 one can think of S_p as consisting of those F that can be observed in configurations that are local minimizers in $W^{1,p}$. In the example (4.4) we have $S_3 = M^{3\times 3}$, $S_1 \neq M^{3\times 3}$ and can view ∂S_1 as a fracture surface. Note, however, that deformations in which x is discontinuous across a plane do not belong to $W^{1,1}(\Omega;\mathbb{R}^3)$, and therefore that the above framework cannot handle the most common type of fracture; this may not be as serious as it sounds, as there is evidence that in some materials cracks are initiated by cavitation. For another speculative approach to the onset of fracture see Ball & Mizel [8].

As a final result concerning quasiconvexity we mention the recent beautiful theorem of Knops & Stuart [22] which states that if W is strictly $W^{1,\infty}$-quasiconvex and C^1 for $\det F > 0$ then for zero body forces the only smooth solution of the equilibrium equations

$$\frac{\partial}{\partial X^\alpha} \frac{\partial W}{\partial x^i_{,\alpha}} = 0 \quad \text{in } \bar{\Omega}$$

satisfying $\det \nabla x(X) > 0$ in $\bar{\Omega}$ and the homogeneous boundary data

$$x(X)\Big|_{\partial\Omega} = AX$$

is $x(X) \equiv AX$, provided Ω is star-shaped.

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