Lyapunov Functions for Thermomechanics with Spatially Varying Boundary Temperatures

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Dedicated to James Serrin on the occasion of his 60th birthday

1. Introduction

Consider a continuous body subjected to conservative body and surface forces, with a part $\partial\Omega_2$ of the boundary maintained at a temperature $\theta = \theta_0(X)$ and with the remainder of the boundary thermally insulated. A calculation of DUHEM [1911] shows that if θ_0 is *constant* then the equations of motion possess a Lyapunov function, the *equilibrium free energy*, given in a standard notation (see Section 2) by

$$E = \int_\Omega \varrho_R(\tfrac{1}{2}|v|^2 + U + \psi - \theta_0\eta)\, dX - \int_{\partial\Omega\setminus\partial\Omega_1} t_R \cdot x\, dA. \tag{1.1}$$

The purpose of this paper is to show that for certain cases when the reference heat flux vector $q_R = \hat{q}_R(X, \theta, \text{Grad}\,\theta)$ there is a corresponding equilibrium free energy function, namely

$$E = \int_\Omega \varrho_R(\tfrac{1}{2}|v|^2 + U + \psi - \phi(X)\eta)\, dX - \int_{\partial\Omega\setminus\partial\Omega_1} t_R \cdot x\, dA, \tag{1.2}$$

that is nonincreasing along solutions even when θ_0 depends on X.

In (1.2) ϕ denotes the solution of the stationary heat equation

$$\text{Div}\, \hat{q}_R(X, \phi, \text{Grad}\,\phi) = 0, \qquad X \in \Omega, \tag{1.3}$$

with boundary conditions

$$\phi|_{\partial\Omega_2} = \theta_0, \qquad \hat{q}_R(X, \phi, \text{Grad}\,\phi) \cdot N|_{\partial\Omega\setminus\partial\Omega_2} = 0. \tag{1.4}$$

In Section 2 we give a formal argument showing that if ϕ is any function satisfying $\phi|_{\partial\Omega_2} = \theta_0$ then, for motions satisfying the Planck inequality we have in general that

$$\dot{E} + I \leq 0, \tag{1.5}$$

where

$$I = \int_\Omega \text{Grad}\left(\frac{\phi}{\theta}\right) \cdot q_R\, dX. \tag{1.6}$$

The argument applies in particular to thermoelasticity, when equality holds in the Planck inequality.

In Section 3 we make a detailed study of the dissipation integral (1.6) with ϕ given by (1.3), (1.4), showing that $I = I(\theta) \geqq 0$ for all temperature distributions $\theta(\cdot)$ satisfying the boundary conditions in the two cases

(a) $\hat{q}_{\mathrm{R}} = -k(\theta)\,\mathrm{Grad}\,\theta$, where $\log k(\theta)$ is a concave function of $\log\theta$,

(b) $\hat{q}_{\mathrm{R}} = -K(X)\,\mathrm{Grad}\,\theta$, where K is a uniformly positive matrix.

In case (a) we show that if $\log k(\theta)$ is sufficiently convex in $\log\theta$ on some interval then $I(\theta)$ can be negative, and hence E is not a Lyapunov function.

In cases when E is a Lyapunov function it is natural to conjecture that successive states of the body at a sequence of times $t_j \to \infty$ will generically realize, in an appropriate sense, a minimizing sequence for the functional E. Consider, for example, a thermoelastic material. If the boundary conditions allow conserved quantities these should be considered as constraints, and it may then happen (*cf.* MAN [1985]) that the velocity fields of minimizing sequences do not tend to zero as $t \to \infty$. Otherwise, however, the preceding motivation leads to consideration of minimization problems for

$$\hat{E}(x) = \int_{\Omega} \varrho_{\mathrm{R}}(X)\,[W(X, Dx(X)) + \psi(X, x(X))]\,dX - \int_{\partial\Omega\setminus\partial\Omega_1} t_{\mathrm{R}} \cdot x\,dA, \tag{1.7}$$

where $W(X, F) \overset{\mathrm{def}}{=} U(X, F, \phi(X)) - \phi(X)\,\eta(X, F, \phi(X))$. Under appropriate hypotheses the study of such minimization problems falls into the framework given in BALL [1977] (see BALL & MURAT [1984] for developments and additional references). For further discussion concerning the relationship between thermodynamics and minimization of $\hat{E}$ see BALL [1984], where the results in this paper were announced, and BALL & KNOWLES [1985].

It would be interesting to find Lyapunov functions for some cases when q_R depends also on mechanical variables and allowing spatially varying boundary temperatures. A Lyapunov function applying to the case when the spatial heat flux vector q is given by

$$q = -k(\theta)\,\mathrm{grad}\,\theta,$$

the gradient being with respect to x, could be relevant for the study of Bénard convection, for example.

2. Equilibrium Free Energy

Consider a continuous body occupying in a reference configuration the bounded open subset $\Omega \subset \mathbb{R}^n$. At time t the particle occupying in the reference configuration the point $X \in \Omega$ has position $x(X, t) \in \mathbb{R}^n$ and temperature $\theta(X, t) > 0$. Assuming the external volumetric heat supply to be zero, the governing equations are

$$\varrho_{\mathrm{R}}\dot{v} = \mathrm{Div}\,T_R + \varrho_{\mathrm{R}} b, \tag{2.1}$$

$$\varrho_{\mathrm{R}}\dot{U} - \mathrm{tr}\,(T_{\mathrm{R}}\dot{F}^T) + \mathrm{Div}\,q_{\mathrm{R}} = 0, \tag{2.2}$$

where $v = \dot{x}$ is the velocity, $\varrho_R(X)$ is the density in the reference configuration, T_R is the Piola-Kirchhoff stress tensor, b is the body force density, U is the internal energy density, $F = Dx(X, t)$ is the deformation gradient and q_R is the (reference) heat flux vector. (Here and below, Div, D and Grad all refer to differentiation with respect to X, dots to differentiation with respect to t.)

We make the thermodynamic assumption that motions of the body satisfy the *Planck inequality* (see TRUESDELL [1984 p. 112])

$$\varrho_R \theta \dot{\eta} \geqq -\mathrm{Div}\, q_R, \tag{2.3}$$

where $\eta(X, t)$ denotes the specific entropy. We recall that the *Clausius-Duhem inequality*

$$\varrho_R \dot{\eta} \geqq -\mathrm{Div}\left(\frac{q_R}{\theta}\right) \tag{2.4}$$

follows from (2.3) and the *Fourier inequality*

$$q_R \cdot \mathrm{Grad}\, \theta \leqq 0. \tag{2.5}$$

For nonsmooth solutions (2.1)–(2.3) must be interpreted in an appropriate weak or distributional sense (*cf.* DAFERMOS [1983]). We suppose that the body force is conservative, so that

$$b(X, t) = -\nabla_x \psi(X, x(X, t)) \tag{2.6}$$

for some potential $\psi(X, x)$.

We impose the following boundary conditions:

Mechanical:

$$\begin{aligned} x &= x_0(X), \quad X \in \partial\Omega_1, \\ T_R N &= t_R(X), \quad X \in \partial\Omega \setminus \partial\Omega_1, \end{aligned} \tag{2.7}$$

Thermal:

$$\begin{aligned} \theta &= \theta_0(X), \quad X \in \partial\Omega_2, \\ q_R \cdot N &= 0, \quad X \in \partial\Omega \setminus \partial\Omega_2. \end{aligned} \tag{2.8}$$

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_0, t_R, θ_0 are given functions.

Let $\phi = \phi(X) \geqq 0$ be a given function satisfying

$$\phi(X) = \theta_0(X), \quad X \in \partial\Omega_2. \tag{2.9}$$

It follows from (2.1)–(2.3) that

$$\frac{\partial}{\partial t}[\varrho_R(\tfrac{1}{2}|v|^2 + U + \psi - \phi\eta)] \leqq \mathrm{Div}\,[v^T T_R] + \left(\frac{\phi}{\theta} - 1\right)\mathrm{Div}\, q_R. \tag{2.10}$$

Using (2.10) and the boundary conditions (2.7), (2.8) we obtain

$$\dot{E} + I \leqq 0, \tag{2.11}$$

where

$$E = \int_\Omega \varrho_R(\tfrac{1}{2}|v|^2 + U + \psi - \phi\eta)\, dX - \int_{\partial\Omega\setminus\partial\Omega_1} t_R \cdot x\, dA, \tag{2.12}$$

and

$$I = \int_\Omega \operatorname{Grad}\left(\frac{\phi}{\theta}\right) \cdot q_R \, dX. \tag{2.13}$$

Thus E will be nonincreasing along solutions provided

$$I \geqq 0. \tag{2.14}$$

An important special case is when $\theta_0 > 0$ is independent of X. Choosing $\phi \equiv \theta_0$ we find that

$$I = -\theta_0 \int_\Omega \frac{q_R \cdot \operatorname{Grad} \theta}{\theta^2} \, dX, \tag{2.15}$$

so that (2.14) holds provided (2.5) does. In fact in this case $I \geqq 0$ if we assume that (2.4) holds instead of (2.3). This result is well known (see DUHEM [1911], ERICKSEN [1966], COLEMAN & DILL [1973], for example). The corresponding function

$$E = \int_\Omega \varrho_R(\tfrac{1}{2}|v|^2 + U + \psi - \theta_0 \eta) \, dX - \int_{\partial\Omega \setminus \partial\Omega_1} t_R \cdot x \, dA \tag{2.16}$$

is commonly called the *equilibrium free energy*, and we carry over the same terminology to E given by (2.12) whenever ϕ is chosen so that (2.14) holds.

As an example we consider a thermoelastic material, whose constitutive relations are given in terms of the Helmholtz free energy function $A(X, F, \theta)$ by

$$\begin{gathered} T_R = \varrho_R \frac{\partial A}{\partial F}, \quad \eta = -\frac{\partial A}{\partial \theta}, \quad U = A + \eta\theta, \\ q_R = \hat{q}_R(X, F, \theta, \operatorname{Grad} \theta). \end{gathered} \tag{2.17}$$

By (2.2), (2.17) we see, as is well known, that equality holds in (2.3) and that (2.4) reduces to (2.5).

3. The Dissipation Integral

In this section we discuss the positivity of the dissipation integral

$$I(\theta) = \int_\Omega \operatorname{Grad}\left(\frac{\phi}{\theta}\right) \cdot \hat{q}_R(X, \theta, \operatorname{Grad} \theta) \, dX \tag{3.1}$$

given by (2.13) when $q_R = \hat{q}_R(X, \theta, \operatorname{Grad} \theta)$. In (3.1) the admissible functions $\theta > 0$ satisfy the boundary conditions (2.8). We choose ϕ to be a solution of the stationary heat equation

$$\operatorname{Div} \hat{q}_R(X, \phi, \operatorname{Grad} \phi) = 0, \qquad X \in \Omega \tag{3.2}$$

subject to the same boundary conditions

$$\begin{gathered} \phi = \theta_0(X), \qquad X \in \partial\Omega_2, \\ \hat{q}_R(X, \phi, \operatorname{Grad} \phi) \cdot N = 0, \qquad x \in \partial\Omega \setminus \partial\Omega_2. \end{gathered} \tag{3.3}$$

In the examples treated below (3.2) is elliptic and ϕ unique. Proceeding formally for a moment, we observe that the Euler-Lagrange equation for I can be written

$$\frac{\partial}{\partial X^\alpha}\left(\operatorname{Grad}\left(\frac{\phi}{\theta}\right)\cdot\frac{\partial \hat{q}_R}{\partial \theta_{,\alpha}}-\frac{\phi}{\theta^2}\hat{q}_R^\alpha\right)=\operatorname{Grad}\left(\frac{\phi}{\theta}\right)\cdot\frac{\partial \hat{q}_R}{\partial \theta}$$

$$+\hat{q}_R\cdot\left(\frac{2\phi}{\theta^3}\operatorname{Grad}\theta-\frac{1}{\theta^2}\operatorname{Grad}\phi\right). \tag{3.4}$$

It is easily seen that $\theta=\phi$ is a solution of (3.4), and 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 minimizer of I. The problem is not straightforward since ϕ is only known implicitly and the integrand may be negative.

For the remainder of this section we make the technical assumptions that Ω has a sufficiently regular boundary (it is enough that Ω is strongly Lipschitz in the sense of MORREY [1966 Section 3.4]) and that $\partial\Omega_2\subset\partial\Omega$ is closed with positive $(n-1)$-dimensional measure. We suppose further that $\theta_0:\partial\Omega_2\to\mathbb{R}$ is sufficiently regular, specifically that θ_0 is the boundary value on $\partial\Omega_2$ in the sense of trace of some function $\tilde{\theta}\in H^1(\Omega)$, and that there are constants m, M such that

$$0<m\leqq\theta_0(X)\leqq M<\infty\qquad\text{for a.e. } X\in\partial\Omega_2. \tag{3.5}$$

We define a set $\mathscr{A}$ of admissible functions by

$$\mathscr{A}=\Big\{\theta\in H^1(\Omega)\cap L^\infty(\Omega):\operatorname*{ess\,inf}_{X\in\Omega}\theta(X)>0,$$

$$\theta|_{\partial\Omega_2}=\theta_0\quad\text{in the sense of trace}\Big\}.$$

We consider first the case

$$\hat{q}_R=-k(\theta)\operatorname{Grad}\theta, \tag{3.6}$$

where the thermal conductivity $k(\theta)$ is real-valued, continuous and strictly positive for all $\theta>0$. By (3.1), (3.6)

$$I(\theta)=-\int_\Omega k(\theta)\operatorname{Grad}\left(\frac{\phi}{\theta}\right)\cdot\operatorname{Grad}\theta\,dX. \tag{3.7}$$

Writing $\varkappa(\theta)=\int_1^\theta k(s)\,ds$, $g(X)=\varkappa(\theta(X))$, we see that (3.2), (3.3) become

$$\begin{gathered}\Delta g=0\quad\text{in }\Omega,\\ g|_{\partial\Omega_2}=\varkappa(\theta_0),\qquad \left.\frac{\partial g}{\partial n}\right|_{\partial\Omega\setminus\partial\Omega_2}=0.\end{gathered} \tag{3.8}$$

It is easily checked that $\varkappa(\theta_0)$ is the boundary value of an $H^1(\Omega)$ function (for example of $\varkappa(\tilde{\psi})$, where $\tilde{\psi}=\max\{m,\min\{M,\tilde{\theta}\}\}$. It follows by standard theory that (3.8) has a unique weak solution g, i.e. $g\in H^1(\Omega)$, $g|_{\partial\Omega_2}=\varkappa(\theta_0)$, and

$$\int_\Omega\operatorname{Grad}g\cdot\operatorname{Grad}v\,dX=0 \tag{3.9}$$

for all $v \in H^1(\Omega)$ with $v|_{\partial\Omega_2} = 0$. Defining $\phi = \varkappa^{-1}(g)$ we have that

$$\int_\Omega k(\phi) \operatorname{Grad} \phi \cdot \operatorname{Grad} v \, dX = 0 \tag{3.10}$$

for all $v \in H^1(\Omega)$ with $v|_{\partial\Omega_2} = 0$. By the maximum principle (for an appropriate version see CHICCO [1970])

$$m \leqq \phi(X) \leqq M \quad \text{a.e. } X \in \Omega. \tag{3.11}$$

Also $\phi \in C^1(\Omega)$.

Theorem 3.1. *Let* $\log k(\theta)$ *be a concave function of* $\log \theta$. *Then* $I(\theta) \geqq 0$ *for all* $\theta \in \mathscr{A}$.

To prove the theorem we need some elementary lemmas.

Lemma 3.2. *Let Q be an open interval (finite, semi-infinite, or infinite) of* $\mathbb{R}$. *Let* $h: Q \to (0, \infty)$. *Define* $f: Q \times \mathbb{R}^n \to \mathbb{R}$ *by*

$$f(w, y) = \frac{|y|^2}{h(w)}.$$

Then f is convex if and only if h is concave.

Proof. Let $t \in [0, 1]$, $w, \overline{w} \in Q$, $y, \overline{y} \in \mathbb{R}^n$. Then

$$\begin{aligned}
\delta f &\overset{\text{def}}{=} f(tw + (1-t)\overline{w}, ty + (1-t)\overline{y}) - tf(w, y) - (1-t) f(\overline{w}, \overline{y}) \\
&= \frac{1}{h(tw + (1-t)\overline{w})} \Bigg[[th(w) + (1-t) h(\overline{w}) - h(tw + (1-t)\overline{w})] \\
&\quad \times \left(\frac{t|y|^2}{h(w)} + \frac{(1-t)|\overline{y}|^2}{h(\overline{w})} \right) - \frac{t(1-t)}{h(w)\, h(\overline{w})} |h(\overline{w})\, y - h(w)\, \overline{y}|^2 \Bigg].
\end{aligned}$$

If h is concave then clearly $\delta f \leqq 0$, hence f convex. If f is convex the concavity of h follows from $\delta f \leqq 0$ on choosing $\overline{y} = \frac{h(\overline{w})}{h(w)} y$. □

We introduce the change of variable

$$w = \int_1^\theta \frac{k(s)}{s} \, ds \tag{3.12}$$

Let $\theta = \theta(w)$ denote the inverse function; thus $\theta(\cdot): Q \to \mathbb{R}$, where

$$Q = \left(-\int_0^1 \frac{k(s)}{s} \, ds, \quad \int_1^\infty \frac{k(s)}{s} \, ds \right).$$

Lemma 3.3. $k(\theta(\cdot))$ is concave on Q if and only if $\log k(\theta)$ is a concave function of $\log \theta$.

Proof. Suppose $\log k(\theta)$ is concave in $\log \theta$. Then $\log k(\theta)$ is locally Lipschitz in $\log \theta$ on $\mathbb{R}$, and hence $k(\theta)$ is locally Lipschitz in θ on $(0, \infty)$. In particular k is differentiable a.e. on $(0, \infty)$ with locally bounded derivative. By the chain rule the locally Lipschitz function $k(\theta(\cdot))$ has derivative

$$\frac{dk(\theta(w))}{dw} = \frac{d \log k(\theta(w))}{d \log \theta(w)} \quad \text{a.e. } w \in Q. \tag{3.13}$$

Since $d \log k(\theta)/d \log \theta$ is a.e. nonincreasing in $\log \theta$, $dk(\theta(w))/dw$ is a.e. nonincreasing in w. Hence $k(\theta(\cdot))$ is concave.

The converse is proved similarly. □

Remark. By making the identification $h(t) = k(e^t)$, $t = \log \theta$ and using a similar proof one can show that a necessary and sufficient condition for a function $h: \mathbb{R} \to (0, \infty)$ to be such that $\log h(\cdot)$ is convex (respectively concave) is that h be locally integrable and for each $s \in \mathbb{R}$ there exists $\lambda(s) \in \mathbb{R}$ with

$$h(t) \geqq h(s) + \lambda(s) \int_s^t h(\tau)\, d\tau \qquad \text{for all } t \in \mathbb{R},$$

(respectively $\leqq$).

Proof of Theorem 3.1. Let $\theta \in \mathscr{A}$. Then $w = w(X)$ defined by (3.12) belongs to $H^1(\Omega) \cap L^\infty(\Omega)$ with $\operatorname{Grad} w(X) = (k(\theta(X))/\theta(X)) \operatorname{Grad} \theta(X)$ a.e. $X \in \Omega$. Thus $I(\theta) = J(w)$, where

$$J(w) = \int_\Omega \hat{f}(X, w(X), \operatorname{Grad} w(X))\, dX, \tag{3.14}$$

and

$$\hat{f}(X, w, y) \overset{\text{def}}{=} \frac{\phi(X)}{k(\theta(w))} |y|^2 - y \cdot \operatorname{Grad} \phi(X). \tag{3.15}$$

It follows from Lemmas 3.2, 3.3 that $\hat{f}(X, \cdot, \cdot)$ is convex on $I \times \mathbb{R}^n$. Define

$$\overline{w}(X) = \int_1^{\phi(X)} \frac{k(s)}{s}\, ds.$$

Note that $\hat{f}(X, \cdot, \cdot)$ is differentiable at (w, y) unless $y \neq 0$ and $\theta(w)$ belongs to the set S of points where $k(\cdot)$ is not differentiable. Since $\log k(\theta)$ is concave in $\log \theta$, it follows easily that S is countable. If $\phi(X) = s \in S$ on a set M of positive measure then (Morrey [1966 p. 69]) $\operatorname{Grad} \phi(X) = 0$ a.e. $X \in M$. Thus $\hat{f}(X, \cdot, \cdot)$ is differentiable at $(\overline{w}(X), \operatorname{Grad} \overline{w}(X))$ for a.e. $X \in \Omega$, and by the convexity we have

$$(\hat{f}X, w(X), \operatorname{Grad} w(X)) \geqq \hat{f}(X, \overline{w}(X), \operatorname{Grad} \overline{w}(X)) + r_w(X), \qquad \text{a.e. } X \in \Omega, \tag{3.16}$$

where

$$r_w(X) = \frac{\partial \hat{f}}{\partial w}(X, \overline{w}(X), \text{Grad}\, \overline{w}(X))\,(w(X) - \overline{w}(X))$$

$$+ \frac{\partial \hat{f}}{\partial y}(X, \overline{w}(X), \text{Grad}\, \overline{w}(X)) \cdot (\text{Grad}\, w(X) - \text{Grad}\, \overline{w}(X))$$

$$= -\frac{k'(\phi)}{k(\phi)} |\text{Grad}\, \phi|^2 \int_\phi^\theta \frac{k(s)}{s}\, ds + \text{Grad}\, \phi \cdot \text{Grad}\left(\int_\phi^\theta \frac{k(s)}{s}\, ds\right),$$

since $\theta(\overline{w}(X)) = \phi(X)$. Setting $u = \int_\phi^\theta \frac{k(s)}{s}\, ds$, $cv = \frac{u}{k(\phi)}$ and noting that since $k(\cdot)$ is Lipschitz, $v \in H^1(\Omega)$ (*cf.* MARCUS & MIZEL [1972]) with $v|_{\partial\Omega_2} = 0$, we deduce from (3.10) that

$$\int_\Omega r_w(X)\, dX = 0. \tag{3.17}$$

Integrating (3.16) we thus have $I(\theta) \geqq I(\phi) = 0$ as required. □

Remark. The proof in fact shows that $I(\theta) \geqq 0$ for all $\theta \in \mathscr{A}_1$, where $\mathscr{A}_1 = \{\theta \in W^{1,1}(\Omega) : \theta > 0$ a.e., $w = \int_1^\theta \frac{k(s)}{s}\, ds \in H^1(\Omega)$ and $\theta|_{\partial\Omega_2} = \theta_0$ in the sense of trace$\}$.

The condition that $\log k$ be concave in $\log \theta$ is satisfied, for example, by the functions

$$k(\theta) = \mu\theta^\alpha, \quad \mu > 0, \quad \alpha \in \mathbb{R},$$

$$k(\theta) = \mu (\log \theta)^\alpha, \quad \mu > 0, \quad \alpha > 0,$$

the first example (for applications see KATH & COHEN [1982], LARSEN & POMRANING [1980], ZELDOVICH & RAIZER [1969]) being critical in that $\log k$ is affine in $\log \theta$. Clearly products of k's satisfying the condition also satisfy it. If k is C^1 on $(0, \infty)$ the condition takes the form that $\theta k'(\theta)/k(\theta)$ be nonincreasing in θ.

To investigate how close the condition is to being necessary for I to be nonnegative on $\mathscr{A}$ we compute the second variation. Suppose k is C^2 on $(0, \infty)$. Let $u \in W^{1,\infty}(\Omega)$ with $u|_{\partial\Omega_2} = 0$. Then

$$\delta^2 I(\phi)\,(\phi u, \phi u) \stackrel{\text{def}}{=} \frac{d^2}{d\varepsilon^2} I(\phi(1 + \varepsilon u))|_{\varepsilon=0}$$

$$= 2 \int_\Omega \text{Grad}\, u \cdot \text{Grad}\,(\phi k(\phi)\, u)\, dX$$

$$= \int_\Omega [2a\, |\text{Grad}\, u|^2 - \Delta a \cdot u^2]\, dX, \tag{3.18}$$

where $a \overset{\text{def}}{=} \phi k(\phi)$ and where we have used (3.9). Note that

$$\Delta a = \left[\left(\frac{\phi k'(\phi)}{k(\phi)} + 1\right) k(\phi)\, \phi_{,\alpha}\right]_{,\alpha}$$

$$= \left(\frac{\phi k'}{k}\right)' k(\phi)\, |\text{Grad}\, \phi|^2. \tag{3.19}$$

In particular, if $\log k(\theta)$ is concave in $\log \theta$ then $\Delta a \leqq 0$ and $\delta^2 I(\phi) \geqq 0$, consistent with Theorem 3.1. The Jacobi equation, that is the Euler-Lagrange equation for (3.18), is

$$\text{Div}\,(2a\, \text{Grad}\, u) = -\Delta a \cdot u. \tag{3.20}$$

We now let $n = 1$, $\Omega = (0, 1)$, $\partial\Omega_2 = \partial\Omega$, so that

$$k(\phi)\, \phi_X = c, \qquad X \in [0, 1], \tag{3.21}$$

where we assume $c = \varkappa(\theta_0(1)) - \varkappa(\theta_0(0))$ is nonzero. We seek a function $u(X) = z(\tau)$, $\tau = \log \phi$, making (3.18) negative. Note that for such a function, by (3.19), (3.21),

$$\delta^2 I(\phi)\, (\phi u, \phi u) = J(z),$$

where

$$J(z) = 2c \int\limits_{\log\theta_0(0)}^{\log\theta_0(1)} [z_\tau^2 - \tfrac{1}{2} p(\tau)\, z^2]\, d\tau \tag{3.22}$$

and

$$p(\tau) = \frac{d^2}{d\tau^2} \log k(e^\tau). \tag{3.23}$$

Also, (3.20) becomes

$$z_{\tau\tau} + \tfrac{1}{2} p(\tau)\, z = 0. \tag{3.24}$$

Suppose that we can find a solution $\bar{z} \neq 0$ of (3.24) on an interval $[\alpha, \beta]$ with $\bar{z}(\alpha) = \bar{z}(\beta) = 0$. Let

$$\theta_0(0) < e^\alpha, \qquad \theta_0(1) > e^\beta. \tag{3.25}$$

Employing classical reasoning (*cf.* BOLZA [1904]) we set

$$z_1(\tau) = \begin{cases} \bar{z}(\tau), & \tau \in [\alpha, \beta], \\ 0 & \text{otherwise}, \end{cases}$$

and note that by (3.24)

$$J(z_1) = 2c \int\limits_\alpha^\beta [\bar{z}_\tau^2 - \tfrac{1}{2} p(\tau)\, \bar{z}^2]\, d\tau$$

$$= 2c \bar{z} \bar{z}_\tau \big|_\alpha^\beta = 0.$$

But z_1 cannot be a minimizer of J among $W^{1,\infty}$ functions vanishing at $\log \theta_0(0)$, $\log \theta_0(1)$ since by standard arguments z_1 would then be a smooth solution of (3.24) on $[\log \theta_0(0), \log \theta_0(1)]$. In particular we would have $\bar{z}_\tau(\alpha) = 0$, and hence

$\bar{z} \equiv 0$ by uniqueness of solutions to the initial-value problem for (3.24), a contradiction. Thus $J(z)$ takes negative values and so

$$\inf_{\theta \in \mathscr{A}} I(\theta) < I(\phi) = 0. \tag{3.26}$$

We give two ways of constructing an appropriate solution $\bar{z}$. First, suppose $\log k(\theta)$ convex in $\log \theta$ but not affine, equivalently $\theta k'(\theta)/k(\theta)$ nondecreasing in θ but not constant. Then $p(\tau) \geqq 0$ and $p(\tau_0) > 0$ for some τ_0. Let $\bar{z}$ be the solution of (3.24) with initial data $\bar{z}(\tau_0) = 1$, $\bar{z}_\tau(\tau_0) = 0$. Since $\bar{z}_{\tau\tau} \leqq 0$ where $\bar{z} \geqq 0$ and since $\bar{z}_{\tau\tau}(\tau_0) < 0$ it follows that $\bar{z}$ has two roots α, β with $\alpha < \tau_0 < \beta$. Second, suppose that $p(\tau) \geqq 2\varepsilon^2 > 0$ on an interval of length greater than π/ε. If τ_0 is the mid-point of the interval and $\bar{z}$ is the solution of (3.24) with $\bar{z}(\tau_0) = 1$, $\bar{z}_\tau(\tau_0) = 0$ then $\bar{z}$ has at least two zeros in $[\tau_0 - \pi/2\varepsilon, \tau_0 + \pi/2\varepsilon]$; this follows from Sturm's first comparison theorem (HARTMAN [1964] p. 334) using the comparison solution $w = \cos \varepsilon(\tau - \tau_0)$ of $w_{\tau\tau} + \varepsilon^2 w = 0$.

If $n > 1$ and either of the above two conditions on k holds then by choosing $\Omega = (0, 1) \times \Omega'$, where Ω' is a bounded open subset of $\mathbb{R}^{n-1}$, and $\partial\Omega_2 = \{0,1\} \times \Omega'$ we can find a function $\theta = \theta(X^1)$ in $\mathscr{A}$ satisfying (3.26). We have thus proved

Theorem 3.4. *Let* $n \geqq 1$. *Suppose* k *is* C^2 *on* $(0, \infty)$ *and satisfies either*

(i) $\log k(\theta)$ *is convex in* $\log \theta$ *but not affine, or*

(ii) $\dfrac{d^2 \log k(\theta)}{d(\log \theta)^2} \geqq 2\varepsilon^2 > 0$ *on an interval of length greater than* $\dfrac{\pi}{\varepsilon}$.

Then we can find Ω, $\partial\Omega_2$, θ_0 *such that*

$$\inf_{\theta \in \mathscr{A}} I(\theta) < 0.$$

As an example satisfying both (i) and (ii) one can choose $k(\theta) = e^\theta$. Note that even when (i) or (ii) hold the second variation for some boundary conditions may be positive; if so the field theory of the calculus of variations (see MORREY [1966 p. 12]) can be applied to conclude that ϕ is a strong local minimizer of I, so that E is a Lyapunov function for solutions with $\sup_{t \geq 0} \|\theta(\cdot, t) - \phi(\cdot)\|_{L^\infty(\Omega)}$ sufficiently small. This information might be useful for stability studies.

We consider next the anisotropic linear case

$$\hat{q}_R = -K(X) \operatorname{Grad} \theta, \tag{3.27}$$

where we assume that the matrix K is bounded and measurable in Ω and satisfies

$$K^{\alpha\beta}(X)\, \xi_\alpha \xi_\beta \geqq k_0\, |\xi|^2, \quad \xi \in \mathbb{R}^n, \quad \text{a.e. } X \in \Omega, \tag{3.28}$$

for some constant $k_0 > 0$. We do not need to assume K is symmetric (the Onsager relations, for a critique see TRUESDELL [1984 Lecture 7]). By definition, a weak solution of (3.2), (3.3) is a function $\phi \in H^1(\Omega)$ satisfying $\phi|_{\partial\Omega_2} = \theta_0$ and

$$\int_\Omega K^{\alpha\beta} \phi_{,\beta} v_{,\alpha}\, dX = 0 \tag{3.29}$$

for all $v \in H^1(\Omega)$ with $v|_{\partial\Omega_2} = 0$. It follows from CHICCO [1970] (see also TRUDINGER [1977]) that there exists a unique such weak solution ϕ and that

$$m \leqq \phi(X) \leqq M \quad \text{a.e. } X \in \Omega. \tag{3.30}$$

Defining ϕ in this way, we have from (3.1), (3.27) that

$$I(\theta) = \int_\Omega -\left(\frac{\phi}{\theta}\right)_{,\alpha} K^{\alpha\beta}\theta_{,\beta}\, dX. \tag{3.31}$$

Theorem 3.5. $I(\theta) \geqq 0$ *for all* $\theta \in \mathscr{A}$.

Proof. Let $\theta \in \mathscr{A}$ and define $w = \log\theta - \log\phi$. Then $w \in H^1(\Omega) \cap L^\infty(\Omega)$ with $\operatorname{Grad} w = (1/\theta)\operatorname{Grad}\theta - (1/\phi)\operatorname{Grad}\phi$ a.e. in Ω. Hence

$$\begin{aligned} I(\theta) &= \int_\Omega [\phi K^{\alpha\beta} w_{,\alpha} w_{,\beta} + K^{\alpha\beta}\phi_{,\beta} w_{,\alpha}]\, dX \\ &\geqq \int_\Omega K^{\alpha\beta}\phi_{,\beta} w_{,\alpha}\, dX = 0, \end{aligned}$$

where we have used (3.28) and (3.29). □

Remark. The proof in fact shows that $I(\theta) \geqq 0$ for all $\theta \in \mathscr{A}_2$, where $\mathscr{A}_2 = \{\theta \in H^1(\Omega) : \theta > 0 \text{ a.e., } \log\theta \in H^1(\Omega) \text{ and } \theta|_{\partial\Omega_2} = \theta_0 \text{ in the sense of trace}\}$.

Setting in particular $T_R = 0$, $U = \theta$ in (2.1), (2.2) we see that by Theorems 3.1, 3.5 and under the hypotheses of these theorems

$$\frac{d}{dt}\int_\Omega \varrho_R\,(\theta - \phi\log\theta)\, dX \leqq 0 \tag{3.32}$$

for sufficiently regular positive solutions θ, satisfying $\theta|_{\partial\Omega_2} = \theta_0$, $\left.\frac{\partial\theta}{\partial n}\right|_{\partial\Omega\setminus\partial\Omega_2} = 0$, of the heat equations

$$\varrho_R \frac{\partial\theta}{\partial t} = \operatorname{Div}(k(\theta)\operatorname{Grad}\theta), \tag{3.33}$$

$$\varrho_R \frac{\partial\theta}{\partial t} = \operatorname{Div}(K(X)\operatorname{Grad}\theta), \tag{3.34}$$

respectively. Various Lyapunov functions similar to (3.32) have been used for systems of reaction-diffusion equations, (see ROTHE [1984]).

We end by noting that the hypothesis of *strict* positivity of θ_0 in Theorems 3.1, 3.5 is essential. In fact, if $\hat{q}_R = -\operatorname{Grad}\theta$, $n = 1$, $\Omega = (0, 1)$, $\partial\Omega_2 = \partial\Omega$, $\theta_0(0) = 0$, $\theta_0(1) = 1$, then $\phi(X) = X$ but for $\theta = X^\alpha$, $0 < \alpha < 1$, we have

$$I(\theta) = \int_0^1 -\left(\frac{X}{X^\alpha}\right)_X \alpha X^{\alpha-1}\, dX = -\infty.$$

Acknowledgement. The research of J.M.B. was supported by a U.K. Science and Engineering Research Council Senior Fellowship and by visits to the Mathematics Research Center, University of Wisconsin, and the Institute for Mathematics and its Applications, University of Minnesota.

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(Received August 12, 1985)