

Chapter 1

**DYNAMIC ENERGY
MINIMIZATION AND PHASE
TRANSFORMATIONS IN SOLIDS**

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1. Introduction. In this article I discuss the question of how to give a dynamical justification of the variational principles of mechanics and physics. For example, in classical and continuum mechanics it is common to analyse equilibrium problems by seeking a configuration that minimizes an appropriate energy functional; how can this procedure be rationalized on the basis of the behaviour of solutions to the corresponding dynamical equations?

Central to any discussion of these matters is the Second Law of Thermodynamics. A formulation of the Second Law which has earned a fair measure of acceptance by practitioners of continuum thermodynamics, on account of its apparently wide applicability and clear statement, is the *Clausius-Duhem inequality* (for an interesting discussion see Ericksen [25]). Assuming the external volumetric heat supply to be zero, this inequality has the form

$$(1.1) \quad \frac{d}{dt} \int_{\Omega} \rho_R \eta \, dx + \int_{\partial\Omega} \frac{q_R \cdot N}{\theta} \, dA \geq 0,$$

where $\Omega \subset \mathbb{R}^3$ denotes the region occupied by a material body in a reference configuration, η denotes the entropy density, q_R the material heat-flux vector, θ the absolute temperature, $\rho_R = \rho_R(x)$ the mass density in the reference configuration, and $N = N(x)$ the unit outward normal to the boundary $\partial\Omega$. In two important cases this inequality endows the governing equations of a material body with a *Lyapunov function*, i.e. a real-valued function of the state of the system which is nonincreasing in time for motions of the body. The first case is that of a thermally isolated body, when $q_R = 0$ on $\partial\Omega$, so that (1.1) implies that

$$(1.2) \quad \frac{d}{dt} \int_{\Omega} -\rho_R \eta \, dx \leq 0.$$

The second case is that of a body for which part of the boundary $\partial\Omega_1$ is thermally insulated and the remainder is in contact with a heat-bath at temperature θ_0 , where θ_0 does not depend on x but could depend on t . Assume for simplicity that the mechanical boundary conditions do no work. Then combining (1.1) with the energy equation

$$(1.3) \quad \frac{d}{dt} \int_{\Omega} \rho_R \left(\frac{1}{2} |v|^2 + \varepsilon + \psi \right) dx + \int_{\partial\Omega} q_R \cdot N dA = 0,$$

where v denotes the velocity, ε the internal energy density, and ψ the potential energy density of the body-forces, we deduce from (1.1) that

$$(1.4) \quad \frac{d}{dt} \int_{\Omega} \rho_R \left(\frac{1}{2} |v|^2 + \psi + \varepsilon - \theta_0 \eta \right) dx \leq 0,$$

(cf. Duhem [21], Ericksen [22], Coleman & Dill [19], for example). Note that the expression $\varepsilon - \theta_0 \eta$ in (1.4) is not the same as the Helmholtz free energy $\varepsilon - \theta \eta$.

If θ_0 is allowed to depend on x then in general the existence of a Lyapunov function is in doubt. However, in some special cases when $\theta_0 = \theta_0(x)$ and $q_R = \hat{q}_R(x, \theta, \text{Grad } \theta)$ it has been shown by Ball & Knowles [12] that

$$(1.5) \quad \frac{d}{dt} \int_{\Omega} \rho_R \left(\frac{1}{2} |v|^2 + \psi + \varepsilon - \varphi(x) \eta \right) dx \leq 0,$$

where φ is the solution to the steady-state heat problem

$$(1.6) \quad \text{div } \hat{q}_R(x, \varphi, \text{Grad } \varphi) = 0, \quad x \in \Omega,$$

$$(1.7) \quad \varphi|_{\partial\Omega \setminus \partial\Omega_1} = \theta_0, \quad \hat{q}_R(x, \varphi, \text{Grad } \varphi) \cdot N|_{\partial\Omega_1} = 0.$$

There seems to be a wide gulf between modern continuum thermodynamics as expressed, for example, by the balance of energy and the Clausius-Duhem inequality, and nonequilibrium statistical physics and kinetic theory. The Clausius-Duhem inequality is systematically applied with apparent success to a wide range of different materials out of equilibrium, leading to the existence of Lyapunov functions as described above. On the other hand statistical physics provides Lyapunov functions only for very special materials, the main example being the H-theorem for the Boltzmann equation, which models a moderately rarified monatomic gas. One approach to trying to bridge this gulf is to attempt to make precise the idea that in a system of interacting particles local equilibrium is rapidly achieved (cf. Guo, Papanicolaou & Varadhan [28], Varadhan [43]).

With the above as motivation, suppose we are given a dynamical system $T(t)_{t \geq 0}$ on some (say, topological) space X , i.e. a family of mappings $T(t) : X \rightarrow X$ satisfying (i) $T(0) = \text{identity}$, (ii) $T(s+t) = T(s)T(t)$ for all $s, t \geq 0$, (iii) the mapping $(t, \varphi) \mapsto T(t)\varphi$ is continuous. Thus $T(t)\varphi$ represents the state reached by the system after time t starting with initial data φ . Let $V : X \rightarrow \mathbf{R}$ be a continuous Lyapunov function, so that $V(T(t)\varphi)$ is nonincreasing on $[0, \infty)$ for each $\varphi \in X$. In order to justify dynamically the variational principle

$$(1.8) \quad \text{Minimize } V$$

we would like to show that if $t_j \rightarrow \infty$ then $T(t_j)\varphi$ will be a local minimizing sequence (appropriately defined) for V . As described in Ball [5] (of which this article is an updated version), there are various obstacles to proving such a result. Some of these are:

- (a) Exceptional initial data (such as an unstable rest-point) must be excluded.
- (b) There may be constants of motion $c_i : X \rightarrow \mathbf{R}$, so that $c_i(T(t))\varphi = c_i(\varphi)$ for all i and $t \geq 0$; the traditional remedy is then to change the variational principle to

$$(1.9) \quad \begin{aligned} & \text{Minimize } V(\psi) \\ & c_i(\psi) = \alpha_i \end{aligned}$$

(c) Nonhyperbolic rest-points. (For example, $V(x) = -x$ is a Lyapunov function for the ordinary differential equation $\dot{x} = x^2(1 - x^2)$ on $[-1, 1]$. This has the three rest-points $-1, 0, 1$. The rest-point 0 is not hyperbolic and is not a local minimizer of V , but $x(t) \rightarrow 0$ whenever $-1 < x(0) \leq 0$.)

(d) V may not attain a minimum.

As far as I am aware, no sufficiently general theorem for dynamical systems is known that overcomes these obstacles. Some ideas which are of relevance are to be found in the study of prolongational limit sets for dynamical systems (cf. Ura [41,42], Auslander & Seibert [2], Bhatia & Szego [14]), and the behaviour of solutions to differential equations with small random perturbations (see for the finite-dimensional case Freidlin & Wentzell [26], and for results for parabolic partial differential equations forthcoming work of Freidlin). I intend to discuss this in a future paper. In particular, the infinite-dimensional situation is far from being understood, and the main purpose of this article is to discuss some infinite-dimensional examples arising in models for phase transformations in solids, in which (d) is an issue. In these examples the minimum of V is not attained, minimizing sequences for V tending weakly to a state that is not a minimizer.

In Section 2 I consider systems of coagulation-fragmentation equations, and how they model the phenomenon of condensation. Here it is shown that the dynamics realize an absolute minimizing sequence for the free energy. Section 3 concerns a variational approach to the formation of microstructure arising from displacive phase transformations in crystals, while in Section 4 I outline some attempts to understand how this microstructure forms dynamically. Some model problems are discussed which exhibit surprising differences between the asymptotic behaviour of solutions for rather similar systems.

2. Coagulation-fragmentation dynamics. Coagulation-fragmentation equations occur frequently in applications to fields such as astrophysics, atmospheric physics, biology, colloidal chemistry, polymer science and the kinetics of phase transformations in alloys. They are appropriate for many systems in which the objects of interest are a large number of clusters of particles, and model the time-evolution of the distribution of cluster sizes as the clusters coalesce to form larger clusters and fragment to form smaller ones. In the case of phase transformations in a binary alloy, the clusters consist of atoms of the minority component of the alloy (or, in more complex cases, atoms of both components in a definite proportion corresponding to a particular phase of the alloy), and the interactions between clusters occur by diffusion of atoms on the underlying crystal lattice.

We assume that only binary interactions between clusters occur. For example, a 3-cluster (i.e. a cluster consisting of 3 particles) may coalesce with a 7-cluster to form a 10-cluster, or the reverse may occur, a 10-cluster fragmenting into a 3-cluster and a 7-cluster, but we ignore interactions in which, say, a 4-cluster fragments into a 2-cluster and two 1-clusters. Let $c_j = c_j(t) \geq 0, j = 1, 2, \dots$, denote the expected number per unit volume of j -clusters in the system at time t . Assuming that the rate at which j -clusters coalesce with k -clusters to form $(j+k)$ -clusters is proportional both to c_j and c_k , while the rate at which $(j+k)$ -clusters fragment into j -clusters and k -clusters is proportional to c_{j+k} , we are led to the *discrete coagulation-fragmentation equations* for $c = (c_j)$:

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$$(2.10) \quad \dot{c}_j = \frac{1}{2} \sum_{k=1}^{j-1} (a_{j-k,k} c_{j-k} c_k - b_{j-k,k} c_j) - \sum_{k=1}^{\infty} (a_{j,k} c_j c_k - b_{j,k} c_{j+k}),$$

$$j = 1, 2, \dots$$

The rate coefficients $a_{j,k}$, $b_{j,k}$ are assumed to be constant and satisfy the conditions

$$(2.11) \quad a_{j,k} = a_{k,j} \geq 0,$$

$$(2.12) \quad b_{j,k} = b_{k,j} \geq 0.$$

Because each interaction preserves the number of particles, we expect that density will be conserved, i.e.

$$(2.13) \quad \sum_{j=1}^{\infty} j c_j(t) = \rho = \text{constant}.$$

While (2.13) holds formally for solutions of (2.10), it is well known that for some rate coefficients $a_{j,k}$, $b_{j,k}$ density conservation breaks down after a finite time due to the formation of an infinite cluster or gel. Mathematically, the situation is analogous to that for nonlinear hyperbolic equations, for which various entropies which are conserved for smooth solutions fail to be conserved for solutions containing shock waves. Here we confine attention to solutions conserving density. It is proved in Ball & Carr [7] that at least one density-conserving solution exists provided $a_{j,k} \leq K(j+k)$ for all $j, k \geq 1$, where K is a constant. Conditions on $a_{j,k}$, $b_{j,k}$ are also given in [7] under which all solutions conserve density, and under which solutions are unique.

We now assume that the rate coefficients satisfy the *detailed balance* condition

$$(2.14) \quad a_{j,k} Q_j Q_k = Q_{j+k} b_{j,k},$$

for positive constants Q_j with $Q_1 = 1$, and we confine attention to the physically interesting case

$$(2.15) \quad 0 < z_s < \infty,$$

where

$$(2.16) \quad z_s^{-1} = \limsup_{j \rightarrow \infty} Q_j^{1/j}.$$

It is easily verified that for each $z \geq 0$

$$(2.17) \quad c_j = Q_j z^j, \quad j = 1, 2, \dots,$$

is a rest-point of (2.10). In fact, in this case the net rate $W_{j,k} = a_{j,k} c_j c_k - b_{j,k} c_{j+k}$ of conversion of j -clusters and k -clusters to $(j+k)$ -clusters is zero (this being the physical meaning of detailed balancing). To see whether these rest-points have finite density given by (2.13), note that by (2.16) the radius of convergence of the series $F(z) = \sum_{j=1}^{\infty} j Q_j z^j$ is z_s . Let

$$(2.18) \quad \rho_s = \sum_{j=1}^{\infty} j Q_j z_s^j.$$

Then for $0 \leq \rho \leq \rho_s$, $\rho < \infty$, there is a unique rest-point c^ρ of the form (2.17) of density ρ , namely

$$(2.19) \quad c_j = Q_j z(\rho)^j, \quad j = 1, 2, \dots,$$

where $F(z(\rho)) = \rho$.

Let

$$(2.20) \quad V(c) = \sum_{j=1}^{\infty} c_j \left(\ln \left(\frac{c_j}{Q_j} \right) - 1 \right),$$

where $c = (c_j)$. A formal calculation shows that

$$(2.21) \quad \frac{dV}{dt} = -\frac{1}{2} \sum_{j,k=1}^{\infty} (\ln(a_{j,k} c_j c_k) - \ln(b_{j,k} c_{j+k})) (a_{j,k} c_j c_k - b_{j,k} c_{j+k}),$$

so that V is a Liapunov function (the *free energy*). Note that (2.21) shows formally that all rest-points of (2.10) are of the form (2.17).

Since the density (2.13) is a constant of motion, the appropriate variational principle for $c = (c_j) \geq 0$ is

$$(2.22) \quad \begin{array}{l} \text{Minimize } V(c) \\ \sum_{j=1}^{\infty} j c_j = \rho \end{array},$$

where $\rho \geq 0$. If $0 \leq \rho \leq \rho_s$, $\rho < \infty$, then it is easily verified that c^ρ is the unique minimizer of (2.22), and that any minimizing sequence $c^{(k)}$ converges strongly in

$$(2.23) \quad X \stackrel{\text{def}}{=} \{c \geq 0 : \|c\| = \sum_{j=1}^{\infty} j |c_j| < \infty\},$$

to c^ρ . However, if $\rho_s < \rho < \infty$ then the minimum of V subject to $\sum_{j=1}^{\infty} j c_j = \rho$ is *not attained*. In fact, in this case minimizing sequences $c^{(k)}$ for (2.22) converge weak* to c^{ρ_s} in X i.e. $c_j^{(k)} \rightarrow c_j^{\rho_s}$ as $k \rightarrow \infty$ for all j . There is therefore a difference $\rho - \rho_s$ between the density of elements $c^{(k)}$ of the minimizing sequence and the density of the limit c^{ρ_s} . This difference corresponds to the formation as k increases of clusters of arbitrarily large size. In this way the variational principle (2.22) predicts the macroscopic phenomenon of *condensation*. It is of interest to note (see Ball [4]) that this same variational structure occurs in a number of other problems, for example the Thomas-Fermi model of atoms and molecules, the equilibrium of an incompressible fluid above a surface, and an adiabatic model predicting a finite height for the atmosphere. In each case there is a critical parameter value ρ_s such that for $0 < \rho \leq \rho_s$ the minimum of the energy is attained, while for $\rho > \rho_s$ the minimum is not attained, minimizing sequences converging weakly to the minimizer of maximal parameter value ρ_s .

In order to provide a dynamical description of condensation one must show that given initial data $c_0 = (c_{0j})$ of density ρ , the solution c of (2.10) with $c(0) = c_0$ generates a minimizing sequence for (2.22), that is that if $0 \leq \rho \leq \rho_s$, $\rho < \infty$ then $c(t) \rightarrow c^\rho$ strongly in X as $t \rightarrow \infty$, while if $\rho_s < \rho < \infty$ then $c(t) \xrightarrow{*} c^{\rho_s}$ in X as $t \rightarrow \infty$. This has so far only been established in some special cases. For the *Becker-Döring equations*, for which

$$(2.24) \quad a_{j,k} = b_{j,k} = 0 \quad \text{if both } j > 1, k > 1,$$

the result was proved by Ball, Carr & Penrose [8] (for technical refinements see Ball & Carr [6], Slemrod [38]). When all the $a_{j,k}, b_{j,k}$ are nonzero the only result known is that of Carr [17] under hypotheses which imply that $\rho_s = \infty$, so that condensation does not occur. For the general case, parts of the argument for proving the result are available in [7] (for the continuous analogue of (2.10) see Stewart [39]); what is missing is an analogue or substitute for the maximum principle technique used in [8].

3. A variational approach to the formation of fine microstructure in crystals. When cooled below a critical temperature at which a phase transformation involving a change of symmetry occurs, crystals typically develop characteristic patterns of *microstructure*. In the simplest case this consists of many fine parallel bands, in each of which the deformation of the crystal is affine with respect to its original configuration. In some materials (e.g. InTl [13,16]) this microstructure can be observed in optical microscopes, but in others (e.g. NiMn [3]) high resolution electron microscopy is required, and reveals that the bands are sometimes only a few atomic spacings thick.

Why does such microstructure form, and how can its geometric features be predicted? I describe briefly here a variational approach to this question due to Ball & James [10,11] (for related work on the same model see, for example, [18,24,20]). Following Ericksen [23] the crystal is modelled using nonlinear (thermo)elasticity, which allows both for large deformations and nonlinear stress-strain behaviour. While rarely used by metallurgists, this theory is ideally suited to the study of the mechanical properties of crystals since it incorporates in a natural way, and without the inappropriate approximations of linear elasticity, the symmetries arising from the underlying lattice structure of the crystal and invariance to rigid-body rotations. (There is an earlier 'linearized' version of the theory in [10,11], due to Khachaturyan [29,30], Khachaturyan & Shatalov [31] and Roitburd [35,36], which is still nonlinear; for discussions of the relationship between the two theories see Bhattacharya [15], Kohn [32] and [11].)

Configurations of the crystal are described by invertible mappings $y : \Omega \rightarrow \mathbb{R}^3$, where $\Omega \subset \mathbb{R}^3$ is the region occupied by the crystal in a reference configuration. We suppose that Ω is bounded and open with sufficiently smooth boundary $\partial\Omega$. The total elastic energy is given by

$$(3.25) \quad I(y) = \int_{\Omega} W(Dy(x)) dx,$$

where Dy denotes the gradient of y , and W is the free-energy function of the crystal. In order to describe phase transformations it is important to allow W to depend on temperature, but here we assume that the temperature is held constant, and so we suppress this dependence. We temporarily ignore all other contributions to the energy, in particular any energy associated with interfaces across which Dy jumps. For simplicity, consider a problem in which the deformed position of every point of $\partial\Omega$ is specified, so that

$$(3.26) \quad y|_{\partial\Omega} = \bar{y}(\cdot),$$

for a given mapping $\bar{y} : \partial\Omega \rightarrow \mathbb{R}^3$. We now consider the variational principle

$$(3.27) \quad \text{Minimize } I(y) \text{ subject to (3.26).}$$

The key result of the theory is then that for W appropriate for crystals the minimum is in general *not attained*, finer and finer microstructure being needed to get closer and closer to the infimum of I . In this way the static theory explains the occurrence of microstructure as being a natural consequence of the behaviour of minimizing sequences for a problem of the calculus of variations with a non-attained minimum.

To give some insight into why the minimum of (3.27) need not be attained, consider the case of a cubic to tetragonal phase transformation, such as occurs for InTi or NiMn. We suppose that the temperature is less than the transformation temperature, but take for the reference configuration the undistorted high-temperature cubic phase. Then it is natural to assume that the set M of 3×3 matrices A which minimize $W = W(A)$ is given by

$$(3.28) \quad M = SO(3)U_1 \cup SO(3)U_2 \cup SO(3)U_3,$$

where

$$(3.29) \quad U_1 = \text{diag}(\eta_2, \eta_1, \eta_1), \quad U_2 = \text{diag}(\eta_1, \eta_2, \eta_1), \quad U_3 = \text{diag}(\eta_1, \eta_1, \eta_2),$$

and $\eta_1 > 0$, $\eta_2 > 0$ are the lattice parameters of the transformation. The matrices U_i represent linear transformations of a cube into tetragons with sides parallel to the cubic axes, while the factors $SO(3)$ reflect the invariance of W to rigid-body rotations. We suppose without loss of generality that $W(A) = 0$ for $A \in M$. An elementary (but slightly tricky) calculation shows that given any matrix $A \in SO(3)U_1$, say, there are precisely 2 matrices $B \in SO(3)U_2$ and 2 matrices $B \in SO(3)U_3$ which differ from A by a matrix of rank one. Picking one of these 4 matrices we have

$$(3.30) \quad B - A = a \otimes n$$

for some non-zero vectors $a, n \in \mathbb{R}^3$. Thus we can construct a sequence y^ϵ of deformations whose gradients Dy^ϵ take the values A and B alternately in layers normal to n of thicknesses $\lambda\epsilon$ and $(1-\lambda)\epsilon$ respectively, where $0 < \lambda < 1$. Clearly $W(Dy^\epsilon(x)) = 0$ for a.e. $x \in \Omega$. Let $0 \in \Omega$. By adding a suitable constant vector to each y^ϵ we can assume without loss of generality that $y^\epsilon(0) = 0$. Then as $\epsilon \rightarrow 0$, $y^\epsilon \rightarrow (\lambda A + (1-\lambda)B)x$ uniformly in Ω , but Dy^ϵ oscillates, converging only weak* in L^∞ to $\lambda A + (1-\lambda)B$. Suppose now that the boundary data is given by $\bar{y}(x) = (\lambda A + (1-\lambda)B)x$. Of course y^ϵ does not satisfy (3.26), but by modifying y^ϵ in a thin boundary layer near $\partial\Omega$ it is easy to arrange that the modified sequence \tilde{y}^ϵ satisfies (3.26) and that the energy in the boundary-layer tends to zero as $\epsilon \rightarrow 0$, so that $\lim_{\epsilon \rightarrow 0} I(\tilde{y}^\epsilon) = 0$ and \tilde{y}^ϵ is a minimizing sequence. Hence for these boundary conditions $\inf I = 0$. The nontrivial part of the analysis is to show that *any* minimizing sequence must behave like \tilde{y}^ϵ . In fact, it is proved in [11], using the weak continuity properties of Jacobians, that the gradient Dy^ϵ of every minimizing sequence y^ϵ has the same *Young measure* $(\nu_x)_{x \in \Omega}$, namely the constant measure

$$(3.31) \quad \nu_x = \lambda\delta_A + (1-\lambda)\delta_B.$$

Said differently, the values of $Dy^\epsilon(x)$ converge in measure to the set $\{A, B\}$ in such a way that the local volume fractions of points having gradient near A (resp. near B) tends to λ (resp. $1-\lambda$).

For general boundary conditions \bar{y} more complicated microstructure than simple layering seems to be necessary in order to get a minimizing sequence. The constructions in [11] use 'layers within layers'. For example, a minimizing sequence with Young measure

$$(3.32) \quad \nu_x = \lambda[\nu\delta_A + (1-\nu)\delta_B] + (1-\lambda)[\mu\delta_C + (1-\mu)\delta_D]$$

can be constructed by having alternate layers of thicknesses $\lambda\epsilon$ and $(1-\lambda)\epsilon$ respectively, the layers of thickness $\lambda\epsilon$ consisting of sublayers of thicknesses $\nu\epsilon^2$, $(1-\nu)\epsilon^2$ in which $Dy^f(x)$ takes the values A and B , and the layers of thickness $(1-\lambda)\epsilon$ consisting of sublayers of thicknesses $\mu\epsilon^2$, $(1-\mu)\epsilon^2$ in which $Dy^f(x)$ takes the values C and D . In order to achieve compatibility, the matrices $A, B, C, D \in M$ must satisfy the relations

$$(3.33) \quad B - A = a \otimes n, \quad D - C = b \otimes l,$$

$$(3.34) \quad \nu A + (1-\nu)B - [\mu C + (1-\mu)D] = c \otimes m$$

for nonzero vectors a, b, c, l, m, n . Boundary layers are needed near the interfaces between the larger layers. Such microstructures are observed; see, for example, Arlt [1].

The above theory is quite successful, predicting the correct interface orientations in a variety of observed microstructures. It also illuminates some central questions concerning lower-semicontinuity and regularity in the calculus of variations. The theory predicts *infinitely fine* microstructures. This is both a good and a bad feature, good because extremely fine microstructures are commonly observed, and bad because these microstructures are of course not infinitely fine. The conventional explanation for limited fineness is that there is a small amount of interfacial energy which contributes significantly to the total energy of a fine microstructure. Model 1 in the next section suggests the interesting possibility that there could be additional dynamic effects that limit fineness.

4. Dynamics and crystal microstructure. In this section I explore the question of whether appropriate dynamical equations for crystals have the property that solutions produce finer and finer microstructure as time t increases, thus providing a dynamical justification of the variational principle (3.27). This is a difficult question both from the point of view of modelling and of analysis. As regards modelling, it is not clear what dynamics should be assumed (and in particular what dissipation should be associated with the propagation of interfaces), while the analysis of even the simplest models seems to be beyond the scope of existing methods. For example, a simple viscoelastic model, ignoring thermal effects and the influence of anisotropy on dissipation, is given by the system

$$(4.35) \quad \rho_R y_{tt} = \operatorname{div} D_A W(Dy) + \beta \Delta y_t,$$

$$(4.36) \quad y|_{\partial\Omega} = \bar{y},$$

with initial data

$$(4.37) \quad y(x, 0) = y_0(x), \quad y_t(x, 0) = y_1(x),$$

where $\rho_R > 0$ is the density in the reference configuration, $\beta > 0$ is constant, and y_0, y_1 are given functions with $y_0|_{\partial\Omega} = \bar{y}$. Under hypotheses on W appropriate for crystals, Rybka [37] has proved the existence of solutions for the corresponding problem with zero-traction boundary conditions, and his techniques can probably be adapted for (4.36). However, I am not aware of any results concerning the asymptotic behaviour of solutions. A very interesting video of numerical computations of Swart & Holmes [40] for the case when $\Omega = (0, 1)^2 \subset \mathbb{R}^2$, y is a scalar, and W has only a finite number of minimizers, shows in a striking way how microstructure is rapidly generated by solutions.

With a view to gaining insight into models such as (4.35)-(4.37), a study of some prototype one-dimensional models was carried out by Ball, Holmes, James, Pego & Swart [9]. A surprising difference was found between the asymptotic behaviour of solutions in two closely related models. In both models the unknown is a scalar $u = u(x, t)$ defined for $0 \leq x \leq \pi, t \geq 0$.

Model 1 consists of the system

$$(4.38) \quad u_{tt} = (u_x^3 - u_x)_x - \alpha u + \beta u_{xxt},$$

$$(4.39) \quad u(0, t) = u(\pi, t) = 0$$

where $\alpha > 0, \beta > 0$ are constants, with initial conditions

$$(4.40) \quad u(x, 0) = u_0(x), \quad u_t(x, 0) = u_1(x).$$

Writing $w = u_t$, and

$$(4.41) \quad V_1(u, w) = \int_0^\pi \left[\frac{1}{2} w^2 + \frac{1}{4} (u_x^2 - 1)^2 + \frac{\alpha}{2} u^2 \right] dx,$$

a formal calculation shows that solutions to (4.38),(4.39) satisfy

$$(4.42) \quad \frac{d}{dt} V_1(u, u_t) = -\beta \int_0^\pi |u_{xt}|^2 dx \leq 0,$$

so that V_1 is a Lyapunov function. A phase-plane analysis shows that there are uncountably many rest points for (4.38),(4.39). Uncountably many of these are weak relative minimizers of V_1 in $X = W_0^{1,\infty}(0, \pi) \times L^2(0, \pi)$, but none of them are strong relative minimizers, i.e. local minimizers in the energy space $W_0^{1,4}(0, \pi) \times L^2(0, \pi)$. Furthermore, $\inf_{\{u,w\} \in X} V_1(u, w) = 0$ but the minimum is *not attained*. The following theorem is proved in [9] (together with related existence, uniqueness and regularity theorems for (4.38),(4.39)):

THEOREM 4.1. *There is no solution of (4.38),(4.39) with initial data $\{u_0, u_1\} \in X$ such that*

$$(4.43) \quad \lim_{t \rightarrow \infty} V_1(u, u_t) = 0.$$

Thus there is no solution of (4.38),(4.39) which realizes an absolute minimizing sequence for V_1 ! It is conjectured in [9] that in fact every solution converges to a rest point as $t \rightarrow \infty$. Theorem 4.1 and the conjecture are not inconsistent with the possibility that almost every solution converges to a weak relative minimizer of V_1 ; thus a result of the type discussed in the introduction could hold.

In the simpler case when $\alpha = 0$, Pego [33] proved that every solution to (4.38) converges to a rest-point as $t \rightarrow \infty$ when the boundary condition at $x = \pi$ is changed

to that of zero traction, i.e. $\sigma(u_x) + \beta u_{xt} = 0$ at $x = \pi$, where $\sigma(z) = z^3 - z$. However, for this σ and the zero displacement boundary conditions (4.39) it is not known whether every solution converges to a rest-point. If $\alpha = 0$ and we drop the u_{tt} term in (4.38) then (4.38),(4.39) are seen to be equivalent to the equation

$$(4.44) \quad \beta z_t = -\sigma(z) + \frac{1}{\pi} \int_0^\pi \sigma(z) dx$$

for $z = u_x$. Recently, Friesecke [27], following earlier work on a finite-dimensional version of (4.44) by Pego [34], has shown that each solution of (4.44) that is bounded in $L^\infty(\Omega)$ converges boundedly a.e. to a rest-point, provided that σ is C^1 and is not constant on any interval. It remains to be seen whether these methods can be adapted to handle the case of (4.38),(4.39) with $\alpha > 0$.

Model 2 consists of the system

$$(4.45) \quad u_{tt} = (\|u_x\|^2 u_x - u_x)_x - \alpha u + \beta u_{xxt},$$

$$(4.46) \quad u(0, t) = u(\pi, t) = 0$$

where $\alpha > 0, \beta > 0$ are constants, with initial conditions

$$(4.47) \quad u(x, 0) = u_0(x), \quad u_t(x, 0) = u_1(x),$$

which is obtained from (4.38)-(4.40) by replacing the term u_x^3 with the nonlocal expression $\|u_x\|^2 u_x$, where $\|u_x\| = (\int_0^\pi u_x^2 dx)^{\frac{1}{2}}$. Defining

$$(4.48) \quad V_2(u, w) = \int_0^\pi \left[\frac{1}{2} w^2 + \frac{\alpha}{2} u^2 \right] dx + \frac{1}{4} (\|u_x\|^2 - 1)^2,$$

we find that solutions of (4.45),(4.46) satisfy

$$(4.49) \quad \frac{d}{dt} V_2(u, u_t) = -\beta \int_0^\pi |u_{xt}|^2 dx \leq 0.$$

An elementary Fourier analysis shows that there are a countable number of rest-points $\{\psi_k, 0\}$ for (4.45),(4.46). Also $\inf_{\{u, w\} \in X} V_2(u, w) = 0$, where $X = W_0^{1,2}(0, \pi) \times L^2(0, \pi)$ but the minimum is not attained. The following theorem is proved in [9]:

THEOREM 4.2. *X can be written as the disjoint union of two dense sets A_1, A_2 of first and second category respectively. For initial data $\{u_0, u_1\} \in A_1$, $\{u, u_t\}$ converges in X to a rest-point $\{\psi_k, 0\}$ as $t \rightarrow \infty$. For initial data $\{u_0, u_1\} \in A_2$,*

$$(4.50) \quad \lim_{t \rightarrow \infty} V_2(u, u_t) = 0.$$

Thus in contrast to Model 1, the dynamics of Model 2 generically realize an absolute minimizing sequence for V_2 .

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