Nonsmooth analysis and quasi-convexification in elastic energy minimization problems.

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Abstract

We consider an energy minimization problem for a two-component composite with fixed volume fractions. We study two questions. The first is the dependence of the minimum energy on the constraints and parameters. The second is the rigorous justification of the method of Lagrange multipliers for this problem. We are able to treat only cases with periodic or affine boundary condition. We show that the constrained energy is a smooth and convex function of the constraints. We also find that the Lagrange multiplier problem is a convex dual of the problem with constraints. And we show that these two results are closely linked with each other. Our main tools are the Hashin-Shtrikman variational principle and some results from nonsmooth analysis.

1 Introduction.

The elastic energy minimization problem plays an important role in materials sciences. It arises in finding optimal composite materials, in structural optimization problems and in phase transitions in solids.

One usually minimizes the elastic energy under certain constraints, for example, fixing volume fractions of the component materials and macroscopic strain.

A number of methods have been developed to deal with such problems, either by using the constraints in deriving bounds (see e.g. (Allaire and Kohn 1993b), (Gibiansky and Cherkaev 1984), (Gibiansky and Cherkaev 1987), (Kohn 1991), (Lurie and Cherkaev 1986), (Tartar 1985)) or by including them in the objective functional with Lagrange multipliers, (see e.g. (Bendsøe and Kikuchi 1988), (Jog, Haber and Bendsøe 1992), (Kohn and Strang

*This work was done while Y. G. was a student at the Courant Institute.

1986), (Larché and Cahn 1994), (Strang and Kohn 1988)). It should be noted that there is also work on similar optimization problems using a slightly different viewpoint organized around conditions of optimality (see e.g. (Murat and Tartar 1985)). Sometimes in order to deal with an unconstrained problem one may even introduce the related problem with constraints which might be easier to solve, (see e.g. (Allaire and Kohn 1993c)). Three questions arise. The first is the dependence of the minimal energy on the constraints. The second is the dependence of the energy on the Lagrange multipliers. And the third is the relation between these two questions. In the above papers we find no systematic attempt to answer the above questions.

Some of the works manage to overcome the difficulties by ad hoc means whose general nature is not so clear. For example, in (Kohn 1991) and (Larché and Cahn 1994) the two phases of a composite have the same Hooke's law but different stress-free strain. In (Allaire and Kohn 1993c) one of the materials is assumed to be degenerate. These additional assumptions have the effect of considerably simplifying the calculations. In (Kohn and Strang 1986) and (Strang and Kohn 1988) the optimal design problem for 2-D conductivity is considered via the relaxation formulation. There the relaxed functional can be computed explicitly and it has relatively simple structure to allow the detailed analysis. In this paper we study the minimum energy as a function of parameters and constraints in as much generality as we can.

Our particular setting is the elastic energy minimization for a spatially periodic two-component composite material subject to the constant average strain, or for the equivalent optimization problem with affine boundary condition. We use the Hashin-Shtrikman variational principle and nonsmooth analysis to attain our goal. The smoothness and convexity results are stated in theorems 5 and 6. They are crucial in proving the validity of the Lagrange multiplier method for solving the problem with constraints. The exact correspondence between the Lagrange formulation and the problem with constraints is given in theorem 7. In theorem 8 we prove the curious result that the Lagrange energy and constrained energy are in some sense convex duals of one another. We discuss the general nature of some of our results in the last section of this paper.

Though intuitive, the continuity results are not obvious mathematically and have not been proven up to now in any generality. They are important as a mathematical foundation for the connection between the two approaches mentioned above. Another point that we wanted to make is that certain properties of the optimal quantities can be inferred from the variational principles themselves without explicitly solving the problem (To see how tedious that can be, see e.g. (Allaire and Kohn 1993a)).

2 Problem Formulation and Notation.

In this section we pose the problem and introduce the necessary notation.

The elastic properties at every point x of a periodic composite are described by the fourth order tensor (Hooke's law) $C(x/\varepsilon)$ where $C(x)$ is a periodic function on R^n with the period cell $Q = [0,1]^n$, and ε is small. We consider only two-component composite, so $C(x)$ takes just two values C_1 and C_2; the tensor C_i is the elasticity tensor of the i^{th} component material. Let $\chi_i(x/\varepsilon)$ be the characteristic function of a set occupied by the i^{th} component material, so that

$$C(x) = C_1\chi_1(x) + C_2\chi_2(x),$$
$$\chi_1(x) + \chi_2(x) = 1.$$

We assume that the two materials are well-ordered:

$$C_1 < C_2, \tag{2.1}$$

where the inequality is understood in the sense of quadratic forms over the linear space of 2×2 symmetric matrices. There are two reasons to use this hypothesis. The first is that the well-orderedness is primarily responsible for our monotonicity results. The second is being able to use the optimal energy bounds (see theorem 2 below) as developed in (Allaire and Kohn 1993b). However there is no physical reason to use that assumption.

In the limit as $\varepsilon \to 0$ the composite represents a homogeneous elastic body. If the body is subjected to the uniform strain ξ, then the elastic energy density W will also be uniform throughout the body. It is given by a standard variational principle, (see e.g. (Bensoussan, Lions and Papanicolaou 1978)):

$$W = \inf_{e(v)\in\mathcal{E}(\xi)} \int_Q (C(x)e(v), e(v))dx \tag{2.2}$$

where $Q = [0,1]^n$ is the unit period cell and $\mathcal{E}(\xi)$ is a subspace in $L^2(Q)$ of symmetrized gradients with average value ξ:

$$e(v) = \frac{1}{2}(\nabla v + (\nabla v)^t) \tag{2.3}$$

$$\int_Q e(v)dx = \xi. \tag{2.4}$$

The microgeometry is fixed in (2.2).

Obviously the energy W depends on the microstructure. The problem we address is that of minimizing W when the volume fractions of the component materials are fixed, i.e. when the microgeometry is constrained by

$$\int_Q \chi_1(x)dx = \theta. \tag{2.5}$$

Let us denote this minimal value by $QW_\theta(\xi)$:

$$QW_\theta(\xi) = \inf_{<\chi_1>=\theta}\ \inf_{e(v)\in\mathcal{E}(\xi)} \int_Q (C(x)e(v), e(v))dx \tag{2.6}$$

As we have mentioned in the introduction, there is an alternative way of treating this problem. One can accommodate the constraints by the method of Lagrange multipliers, leading to consideration of the Lagrange energy

$$QW_\lambda(\xi) = \inf_{\theta\in[0,1]}\{QW_\theta(\xi) + \lambda\theta\} \tag{2.7}$$

Our goal is to study the dependence of $QW_\theta(\xi)$ and $QW_\lambda(\xi)$ on θ, λ, and ξ, and to analyze the relation between these two functions.

We should note that all the results about $QW_\theta(\xi)$ will remain valid if in (2.6) we use affine boundary conditions $v = \xi x$ instead of the periodic ones. This statement is well-known to experts, however we were not able to find an appropriate reference. The proof of this result is quite simple. Therefore we prove it here for the sake of completeness.

Let Ω be an open bounded subset in R^n. Let us consider the problem with affine boundary condition:

$$AW_\theta(\xi) = \inf_{<\chi_1>=\theta} \inf_{v|_{\partial\Omega}=\xi x} \fint_\Omega (C(x)e(v), e(v))dx.$$

Then the following theorem is true.

Theorem 1 *The minimal values of energy for affine and periodic problems coincide:*

$$AW_\theta(\xi) = QW_\theta(\xi)$$

Proof.
If we fill the domain Ω with the homogeneous optimal periodic composite with effective Hooke's law C^*:

$$(C^*\xi, \xi) = QW_\theta(\xi)$$

then we obtain an inequality

$$AW_\theta(\xi) \leq QW_\theta(\xi).$$

On the other hand we can fill the period cell Q by a countable number of appropriately scaled nonoverlapping copies of Ω. If we preserve the fields inside each copy of Ω, they will provide the test field for the periodic problem (2.6). Because of the special nature of the affine boundary condition the test field will be admissible as displacements do not experience jumps as be go from one copy of Ω to another. Therefore

$$QW_\theta(\xi) \leq AW_\theta(\xi).$$

Which completes the proof.

3 Regularity analysis.

We start our analysis by recalling the results of (Allaire and Kohn 1993b). First let us introduce the notation necessary to formulate the result. For any $k \in S^{n-1}$, let $V(k)$ be the subspace in the space of $n \times n$ symmetric matrices defined by

$$V(k) = \{E = k \otimes \nu + \nu \otimes k, \quad \nu \in R^n\}$$

Let π_V denote the orthogonal projection onto a subspace V in the space of $n \times n$ matrices using the inner product $(A, B) = \mathbf{Tr}(A^T B)$. Define the fourth order tensor $f(k)$ as

$$(f(k)\eta, \eta) = |\pi_{C_1^{1/2}V(k)} C_1^{-1/2}\eta|^2, \tag{3.1}$$

and let

$$g(\eta) = \sup_{|k|=1} (f(k)\eta, \eta). \tag{3.2}$$

Then we have the following, (Allaire and Kohn 1993b):

Theorem 2 *The minimal value of the energy $QW_\theta(\xi)$ has the characterization*

$$QW_\theta(\xi) = (C_1\xi, \xi) + (1-\theta)h(\theta, \xi) \tag{3.3}$$

where

$$h(\theta, \xi) = \sup_\eta \{2(\xi, \eta) - ((C_2 - C_1)^{-1}\eta, \eta) - \theta g(\eta)\}. \tag{3.4}$$

Using this theorem we will study the smoothness of $QW_\theta(\xi)$ via convex and nonsmooth analysis. We will use the following result repeatedly (it follows easily from Corollary 2 of Theorem 2.8.2 of (Clarke 1983)):

Theorem 3 *Let T be compact Hausdorff space. Let $x_0 \in R^n$ and $U(x_0)$ be a neighborhood of x_0 in R^n. Let $f : U(x_0) \times T \to R$ be continuous in t for each $x \in U(x_0)$ and let*

$$F(x) = \sup_{t \in T} f(x, t) \qquad (\inf_{t \in T} f(x, t)) \tag{3.5}$$

Suppose there is a unique $t_0 \in T$ such that $F(x_0) = f(x_0, t_0)$ then

$$\nabla F(x_0) = \nabla_x f(x_0, t_0)$$

if $\nabla_x f(x, t)$ exists and is continuous on $U(x_0) \times V(t_0)$ for some neighborhood $V(t_0)$ of t_0 in T.

Convexity sometimes provides more detailed information about the problem (3.5). If the function f is strictly convex in t, then it is easy to see that the extremal $t(x)$ is necessarily unique, as required for theorem 3. Convexity also provides a regularity result for $t(x)$. The following well-known result uses lower (upper) semicontinuity — a condition weaker than convexity.

Theorem 4 *Let T and $U(x_0)$ be as in the preceding theorem. Let $f : U(x_0) \times T \to R$ be continuous in x for each $t \in T$ and upper (lower) semicontinuous function of its arguments. Suppose for each $x \in U(x_0)$ there is a unique $t(x) \in T$ such that $F(x) = f(x, t(x))$ then $t(x)$ is continuous on $U(x_0)$.*

Since the proof is very short and simple we give it here for the sake of completeness.
Proof. Let $x_j \to x_\infty$. Since T is compact there is a convergent subsequence $t(x_{j_k}) \to t_\infty$. Then, by definition of $t(x_{j_k})$, for all k and $t \in T$

$$f(x_{j_k}, t(x_{j_k})) \geq f(x_{j_k}, t)$$

Thus by upper semicontinuity of f and continuity in x variable we can pass to the limit in the above inequality. So, for all $t \in T$

$$f(x_\infty, t_\infty) \geq f(x_\infty, t).$$

Therefore

$$t_\infty = t(x_\infty)$$

which implies the continuity of $t(x)$. The theorem is proved.

Now we have all we need to prove our regularity results. We start with $QW_\theta(\xi)$ given by (3.3).

Theorem 5
(i) $QW_\theta(\xi)$ is strictly convex in ξ and θ;
(ii) $QW_\theta(\xi)$ is continuously differentiable in ξ and θ.

We remark here that the smoothness and convexity of $QW_\theta(\xi)$ in ξ were proved earlier by Francfort and Marigo in (Francfort and Marigo 1993) (see Remarks 2.2 and 3.3) in two space dimensions.
Proof. (i) First we remark that $h(\theta,\xi)$ given by (3.4) is convex in (θ,ξ) since it is a supremum of linear functions. The strict convexity of $QW_\theta(\xi)$ in ξ is therefore obvious from (3.3). Now let us prove strict convexity in θ. From (3.1) it is easy to show that for any $k \in S^{n-1}$

$$(f(k)\eta,\eta) \geq \gamma|\eta k|^2 \tag{3.6}$$

for some positive constant γ. For example, one can use the well-known fact that

$$|\pi_V x|^2 = \sup_{v\in V} \frac{(x,v)^2}{|v|^2}$$

Thus from (3.2) and (3.6) we obtain that $g(\eta) \geq \gamma|\eta|^2$. We can also observe that $\eta = 0$ is never a maximizer in (3.4). If it were, then for such values of ξ and θ

$$QW_\theta(\xi) = (C_1\xi,\xi).$$

On the other hand it is well known (see e.g. (Milton and Kohn 1988)) that for all $\theta < 1$ and all $\xi \neq 0$

$$QW_\theta(\xi) \geq (H_\theta\xi,\xi) > (C_1\xi,\xi)$$

where

$$H_\theta = (\theta C_1^{-1} + (1-\theta)C_2^{-1})^{-1}$$

is the harmonic mean. It follows then that $g(\eta) > 0$ for the maximizer in (3.4). It follows from this that the function $h(\theta,\xi)$ is strictly monotone in θ. The strict convexity of $QW_\theta(\xi)$ is now easy to prove. Let $F(\theta) = (1-\theta)h(\theta,\xi)$. For any pair θ_1, θ_2

$$F(\frac{\theta_1+\theta_2}{2}) = (1-\frac{\theta_1+\theta_2}{2})h(\frac{\theta_1+\theta_2}{2}) \leq (1-\frac{\theta_1+\theta_2}{2})\frac{h(\theta_1)+h(\theta_2)}{2} =$$

$$\frac{F(\theta_1)+F(\theta_2)}{2} + \frac{h(\theta_1)-h(\theta_2)}{4}(\theta_1-\theta_2) < \frac{F(\theta_1)+F(\theta_2)}{2}$$

(ii) Let us prove the second part of the theorem. First we observe that g is nonnegative, convex and locally Lipschitz continuous since it is a supremum of such functions. Therefore the function under the supremum in (3.4) is strictly concave in η. Thus the conditions of the theorems 3 and 4 are satisfied for (3.4). If $\eta(\theta,\xi)$ denotes the unique maximizer in (3.4) then $h(\theta,\xi)$ is continuously differentiable with

$$\frac{\partial h(\theta,\xi)}{\partial\theta} = -g(\eta(\theta,\xi)) \tag{3.7}$$

$$\nabla_\xi h(\theta,\xi) = 2\eta(\theta,\xi). \tag{3.8}$$

Thus (ii) follows from (3.3), and the theorem is proved.

We now prove the corresponding regularity result for $QW_\lambda(\xi)$.

Theorem 6
(i) $QW_\lambda(\xi)$ is continuously differentiable in ξ;
(ii) $QW_\lambda(\xi)$ is monotone increasing, concave and continuously differentiable in λ.

Proof.
(i) Is the corollary of theorems 3 and 4, whose conditions are satisfied due to the strict convexity of $QW_\theta(\xi)$ in θ.

(ii) $QW_\lambda(\xi)$ is concave in λ as an infimum of linear functions. We will see later that it is strictly concave on a certain subinterval and linear elsewhere. Continuous differentiability in λ is analogous to (i). Moreover, if $\theta(\lambda)$ denotes the unique minimizer in (2.7) then by Theorem 3

$$\frac{\partial QW_\lambda(\xi)}{\partial\lambda} = \theta(\lambda) \geq 0,$$

which gives the desired monotonicity.

In the above proof we introduced a function $\theta(\lambda)$ which provides the connection between a constrained problem and the problem with Lagrange multipliers. It is interesting to study this function in greater detail.

Theorem 7
(i) The function $\theta(\lambda)$ is continuous.
(ii) There exist $0 < \lambda_1 < \lambda_2 < \infty$ such that $\theta(\lambda)$ is strictly monotone decreasing on $[\lambda_1, \lambda_2]$, $\theta(\lambda) = 1$ for all $\lambda \in [0, \lambda_1]$, and $\theta(\lambda) = 0$ for all $\lambda \in [\lambda_2, \infty)$.

Proof.
(i) is the consequence of the proof of the previous theorem. (ii) First we note that for λ large enough

$$QW_\theta(\xi) + \lambda\theta \geq (H_\theta\xi,\xi) + \lambda\theta \geq (C_2\xi,\xi)$$

with equality if and only if $\theta = 0$. Similarly for λ small enough we have

$$\inf_{\theta\in[0,1]}\{QW_\theta(\xi) + \lambda\theta\} \geq \inf_{\theta\in[0,1]}\{(H_\theta\xi,\xi) + \lambda\theta\} = (C_1\xi,\xi) + \lambda$$

with equality if and only if $\theta = 1$.

Now define

$$\lambda_1 = \sup\{\lambda : \ \theta(\lambda) = 1\} > 0$$

and

$$\lambda_2 = \inf\{\lambda : \ \theta(\lambda) = 0\} < \infty$$

By definition of λ_1, λ_2 the minimum in (2.7) is achieved in the interior of [0,1] for all $\lambda \in (\lambda_1, \lambda_2)$. We recall that $QW_\theta(\xi)$ is continuously differentiable. Then

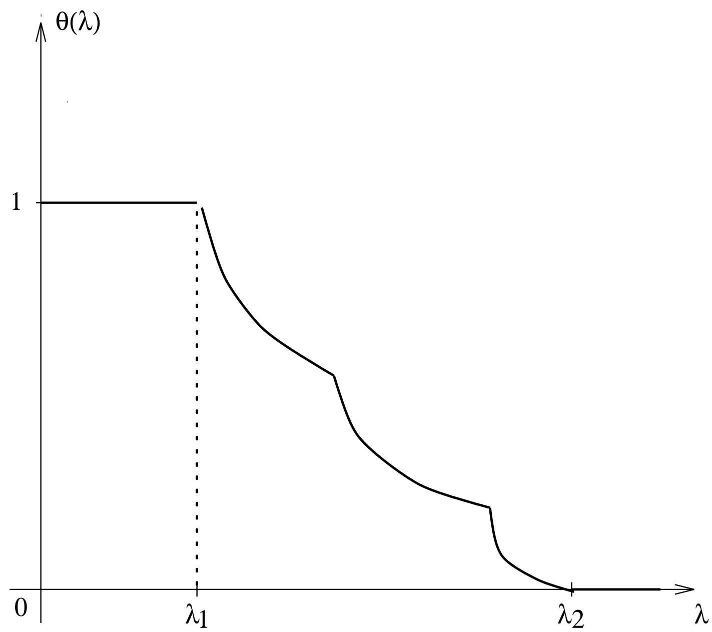
$$\lambda(\theta) = -\frac{\partial QW_\theta}{\partial \theta} \tag{3.9}$$

is continuous. By strict convexity of $QW_\theta(\xi)$ its derivative $-\lambda(\theta)$ is strictly monotone increasing in θ. Thus from (3.9) by inverse function theorem $\theta(\lambda)$ is continuous and strictly monotone decreasing on $[\lambda_1, \lambda_2]$. The theorem is proved.

Corollary 1 *The points λ_1 and λ_2 in the theorem can be found by the following formulas*

$$\left.\begin{aligned} \lambda_1 &= -\frac{\partial QW_\theta(\xi)}{\partial \theta}|_{\theta=1} \\ \lambda_2 &= -\frac{\partial QW_\theta(\xi)}{\partial \theta}|_{\theta=0} \end{aligned}\right\} \tag{3.10}$$

Graphically our results look like this:



Finally, we prove a "duality" result between the constrained energy $QW_\theta(\xi)$ and the Lagrange energy $QW_\lambda(\xi)$.

Theorem 8 *The two functions $QW_\lambda(\xi)$ and $QW_\theta(\xi)$ are related by*

$$QW_\lambda(\xi) = \inf_{\theta \in [0,1]} (QW_\theta(\xi) + \lambda\theta)$$

and

$$QW_\theta(\xi) = \sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta)$$

Proof. The first identity is just a definition of $QW_\lambda(\xi)$. Let us prove the second one. For any λ_0 fixed

$$QW_{\lambda_0}(\xi) = QW_{\theta(\lambda_0)}(\xi) + \lambda_0\theta(\lambda_0)$$

Let λ^* be such that

$$\sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta(\lambda_0)) = QW_{\lambda^*}(\xi) - \lambda^*\theta(\lambda_0))$$

Such a λ^* exists because $QW_\lambda(\xi)$ is bounded and continuous. Then

$$\sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta(\lambda_0)) \geq QW_{\lambda_0}(\xi) - \lambda_0\theta(\lambda_0) = QW_{\theta(\lambda_0)}(\xi) =$$

$$QW_{\theta(\lambda_0)}(\xi) + \lambda^*\theta(\lambda_0) - \lambda^*\theta(\lambda_0) \geq QW_{\lambda^*}(\xi) - \lambda^*\theta(\lambda_0) =$$

$$\sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta(\lambda_0))$$

Comparing the beginning and the end of the chain we see that we have equality everywhere. In particular

$$QW_{\theta(\lambda_0)}(\xi) = \sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta(\lambda_0))$$

But we have shown that any value of θ can be $\theta(\lambda)$ for some λ. Therefore

$$QW_\theta(\xi) = \sup_{\lambda\geq 0}(QW_\lambda(\xi) - \lambda\theta),$$

and the theorem is proved.

4 Final Remarks.

It is interesting to note that the last result of the previous section can be formulated as a convex duality theorem ($f^{**} = f$) and in a broader framework.

Theorem 9 *Let $Q(\theta)$ be convex and monotone decreasing on $[0,1]$. For any $\lambda \geq 0$ let*

$$L(\lambda) = \inf_{\theta\in[0,1]}(Q(\theta) + \lambda\theta).$$

Then $Q(\theta)$ can be recovered from $L(\lambda)$ by the formula

$$Q(\theta) = \sup_{\lambda\geq 0}(L(\lambda) - \lambda\theta)$$

Proof. Let

$$f(x) = \begin{cases} Q(-x) & \text{if } x \in [-1, 0] \\ +\infty & \text{otherwise.} \end{cases}$$

Then it is easy to check that

$$f^*(\lambda) = \begin{cases} -L(\lambda) & \text{for } \lambda > 0 \\ -Q(1) - \lambda & \text{otherwise} \end{cases}$$

since $Q(\theta)$ is monotone decreasing.

By the convexity of $f(x)$ we have

$$Q(\theta) = f(-\theta) = f^{**}(-\theta) = \sup_{\lambda \in R}(-\lambda\theta - f^*(\lambda)).$$

In order to prove the theorem it is sufficient to show that the last supremum can be taken only over $\lambda \geq 0$. Indeed, for $\lambda < 0$ we have

$$-\lambda\theta - f^*(\lambda) = Q(1) + \lambda(1 - \theta) \leq Q(1) = -f^*(0) \leq \sup_{\lambda \geq 0}(-\lambda\theta - f^*(\lambda))$$

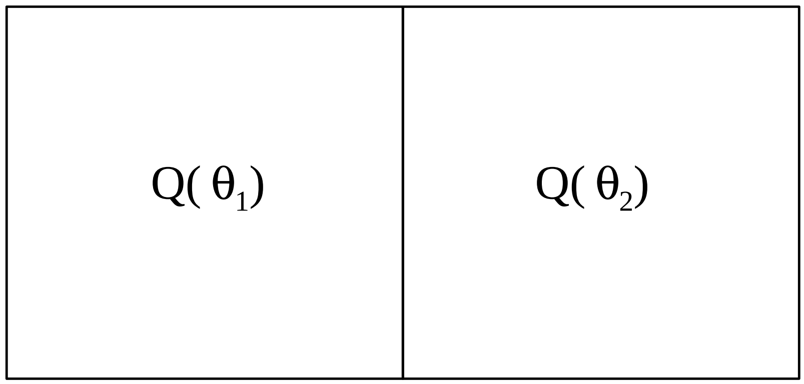
Therefore

$$Q(\theta) = \sup_{\lambda \geq 0}(L(\lambda) - \lambda\theta),$$

and the theorem is proved.

Here we would like to emphasize the particular and the general in the above argument. For example, theorem 9 shows that the conclusion of theorem 8 requires only the knowledge of monotonicity and convexity of the minimal energy as a function of the volume fraction. These properties, as it turns out, have a rather general nature. The monotonicity follows just from the well orderedness assumption (2.1). And convexity is no accident either.

The convexity property is due to the very special — *affine* — boundary condition. In particular for the affine boundary condition the energy density is invariant under translation and scaling. By that we mean that if instead of the domain Ω with $u = \xi x$ on $\partial\Omega$ we considered a different domain $\Omega' = \lambda\Omega + x_0$, where $\lambda > 0$ and $x_0 \in R^n$, with the "same" boundary condition, namely $u = \xi x$ on $\partial\Omega'$, then the energy density would not change. The convexity of $Q(\theta)$ follows now from the additivity of energy (the energy of the system is the sum of energies of all its parts) and the fact that $Q(\theta)$ is an absolute minimum of energies. Indeed, notice first that we can repeat the argument of Theorem 1 using just the above properties to conclude that $Q(\theta)$ does not depend on the domain Ω. Now let us consider the following construction with $u = \xi x$ on all the boundaries:



In the left hand box we put an optimal microstructure corresponding to the volume fraction θ_1 and in the right hand box we put an optimal microstructure corresponding to the volume fraction θ_2. Then the volume fraction for the entire construction is $\theta = (\theta_1 + \theta_2)/2$ and the minimal energy density $Q(\theta)$ is no greater than the energy density of this particular construction. Thus

$$Q(\frac{\theta_1 + \theta_2}{2}) \leq \frac{Q(\theta_1) + Q(\theta_2)}{2},$$

which establishes convexity.

It is natural to ask if our results extend to non-affine boundary condition. For now the situation here is as follows. The well-orderedness condition still provides us with monotonicity. We do not believe the convexity property can be extended as well, since our argument hinges in an essential way on the use of affine (or periodic) boundary condition. Instead of convexity we were able to prove only lower semicontinuity in θ. We conjecture that smoothness properties can be extended under a reasonable assumption on the boundary condition. However, any precise arguments are lacking in this case, yet.

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