Explicit solution of an optimal design problem with non-affine displacement boundary conditions.

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Abstract

Structural optimization problems with non-affine boundary conditions must usually be solved numerically. Here we present an example of such a problem which can be solved *analytically*. Our method utilizes extremal composites as structural components, and makes use of the explicit form of a certain optimal energy bound.

1 Introduction.

A typical problem of optimal design seeks to arrange fixed quantities of given materials within a set $\Omega \in R^n$, so that the resulting structure has an "optimal" response to a particular load. The performance of the design may be measured by some functional of the elastic fields in the structure. Then the goal is to minimize or maximize this functional over all possible geometric arrangements of materials (microstructures).

In this article we consider an optimal material distribution problem, with the objective functional being the strain-energy $\displaystyle\fint_\Omega (C(x)e(u), e(u))dx$. Here $C(x)$ is the local Hooke's law which may take only two values corresponding to two isotropic component materials. The "loading" is produced by prescribing displacement boundary conditions on $\partial\Omega$. **We seek a minimum of the strain energy over all possible phase geometries subject to a constraint on the volume fraction of each phase.** The simplest problem of this type, the problem with affine boundary conditions in two space dimensions, is now rather well understood. Closed form analytical solutions and explicit formulas are available in this case [2], [7], [12], [16], [19]. This paper is different: we consider a problem with *non-affine* boundary conditions.

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To motivate this problem, we observe that it arises in the modeling of precipitation processes due to phase transformations in crystalline solids [13], [14], [15], [17], [22]. In that setting energy minimization is a traditionally accepted mechanism for explaining the shapes of precipitates. We also note that our problem is closely linked with others addressed in the recent literature on optimal design, such as [2], [3], [5], [7], [12], [16], [19], [20], [21]. These articles are concerned with designing "stiff" structures, e.g. by minimizing the complementary energy rather than the elastic energy. In two space dimensions there is a correspondence between problems of elasticity (e.g. plane stress) and plate theory. Elastic energy minimization in the one setting becomes complementary energy minimization in the other. Thus our analysis is directly relevant to the design of stiff plates (see also [7]).

In virtually all cases the solutions to optimal design problems with non-affine boundary conditions have had to be found numerically, at least at the final stage. In this article we present a problem that can be solved *analytically* for a broad class of non-affine Dirichlet data. We must mention that Kohn and Strang have solved explicitly a different problem from two dimensional conductivity with methods and ideas which are very close to ours in all respects [16] (Lemma 8.6). However, we consider our problem in any number of space dimensions, while the previous literature has been focused almost exclusively on the two dimensional case. The formula (3.6) below gives the lower bound on the energy in closed form. Besides being interesting by itself, this explicit solution might be useful as a benchmark, providing a test of any numerical method for solving these structural optimization problems.

The bound we derive is optimal for some but not all choices of the boundary displacements. In this article we obtain necessary and sufficient conditions for the sharpness of the bound in the form of a so called plastic limit analysis problem (see Theorem 1). We solve this problem in the one-dimensional case (see the Appendix), and we also give a necessary condition for the optimality of our bound in the general case (see Proposition 1). The complete characterization of Dirichlet data for which our lower bound is optimal remains an open problem.

Our treatment is based on the use of the homogenization or relaxation technique. In physical terms this means that we are allowed to use composites at every point $x \in \Omega$ in addition to the original materials themselves. This enlargement of the class of admissible structural components does not change the minimum value of the energy, since composites are themselves mixtures of the original materials. On the other hand this enlargement yields a relaxed problem which always has a solution, while the original problem might not have one. The import and mathematical foundation of this idea is discussed in detail in [16], [18]. It is worth mentioning that the task of finding a formula for the relaxed problem is the same as that of solving the optimal design problem with affine boundary conditions [2], [16]. This fact is tacitly used or assumed known in this article and in many references that we cite here.

Our main idea is to use just one of the lower bounds on elastic energy instead of the full form of the relaxed functional (cf. [16] Lemma 8.5). There are several reasons to do this. On the one hand the explicit formula for the relaxed functional is not available in space dimensions more than two (however, see [8] for one simple 3-D case). Even in two space dimensions, where it is available, it is not easily amenable to analysis as it consists of several different lower bounds on the strain energy (three in 2-D), each bound being optimal for a specific range of the average strain (see formula (1.3) of [1]). On the other hand if we decide to use a single bound we can choose the one that is valid for any number of space dimensions (see [9], Chapter 6). Moreover, the Euler-Lagrange equation associated to this bound turns out to be easily solvable.

The drawback of our approach is that a single bound is optimal only for a restricted range of values of the local strain. Therefore, the prescribed boundary displacements must satisfy certain conditions to ensure that the local strain can be chosen in the proper range at every point of the domain. If these conditions are not satisfied, our method is not applicable, and one should resort to numerical computations as was done in [2], [3], [5], [7], [12], [20], [21].

In the next section we introduce our notation and formulate the relaxed problem.

2 Formulation of the relaxed problem.

Let Ω be an open bounded, convex domain in R^n with piecewise smooth boundary. We consider two isotropic materials with bulk and shear moduli denoted by k_i and μ_i respectively. The Hooke's law C_i is then defined by

$$C_i\eta = 2\mu_i\Big(\eta - \frac{1}{n}(\mathbf{Tr}\eta)I\Big) + k_i(\mathbf{Tr}\eta)I \tag{2.1}$$

for any symmetric $n \times n$ matrix η. We shall suppose further that the two materials are well-ordered, i.e. $k_1 > k_2$ and $\mu_1 > \mu_2$; this assumption is necessary for the optimal bound (2.4), (2.5) below to be applicable (see [9]). The total volume of each material is assumed to be given, the first material having the volume $\theta|\Omega|$. The volume fraction θ can be any number between 0 and 1. Also given is the displacement boundary condition $u = g$ on $\partial\Omega$.

We want to minimize the strain energy over all possible microstructures subject to the constraints listed above. The standard energy variational principle allows us to formulate the problem as follows:

$$W_{\min} = \inf_{<\chi>=\theta}\ \inf_{u|_{\partial\Omega}=g} \fint_\Omega \Big(C(x)e(u), e(u)\Big)dx, \tag{2.2}$$

where $C(x)$ is the local Hooke's law

$$C(x) = C_1\chi(x) + C_2(1-\chi(x)),$$

and $e(u)$ is the linear strain

$$e(u) = \frac{1}{2}\Big(\nabla u + (\nabla u)^t\Big).$$

The χ in the outer infimum in (2.2) and in the formula for $C(x)$ denotes the characteristic function of the set occupied by the material **1**, and $< \chi >$ denotes the volume average of the function $\chi(x)$.

The problem (2.2), as is well-known, may not possess a solution in the classical sense, i.e. there might be no characteristic function $\chi(x)$ attaining the infimum in (2.2) [2], [16]. To overcome this difficulty we use the homogenization method discussed in the introduction. It amounts to allowing composites at every point x of Ω. Then instead of $C(x)$ in (2.2) we may use a function $C^*(x)$, which for every x takes its value from $\mathcal{G}_{\theta(x)}$—the set of all effective Hooke's laws that can be obtained by a homogeneous mixture of materials **1** and **2** taken in volume fractions $\theta(x)$ and $1-\theta(x)$. The local volume fraction $\theta(x)$ may take any value from 0 to 1. We only require that $\theta(x)$ be measurable as a function of x and that its volume average be equal to θ. Thus the relaxed problem is

$$W_{\min} = \inf_{<\theta(x)>=\theta} \inf_{u|_{\partial\Omega}=g} \inf_{C^*(x)\in\mathcal{G}_{\theta(x)}} \fint_\Omega \Big(C^*(x)e(u), e(u)\Big)dx. \tag{2.3}$$

It is obvious that at every x it is best to choose $C^*(x)$ to minimize $(C^*(x)e(u), e(u))$ for the given strain $e(u)$ and volume fraction $\theta(x)$. In [9] (section 6) we proved the following inequality for any symmetric $n \times n$ matrix ξ:

$$\inf_{C^*\in\mathcal{G}_\theta} (C^*\xi, \xi) \geq H(k(x) + 2\frac{n-1}{n}\mu_2)(\mathbf{Tr}\xi)^2 - 4\mu_2 J_2(\xi), \tag{2.4}$$

where H denotes the harmonic mean of its argument:

$$H(A(x)) = \Big(\fint_\Omega A^{-1}(x)dx\Big)^{-1}$$

for any invertible tensor $A(x)$, and $J_2(\xi)$ is the second orthogonal invariant of the tensor ξ:

$$J_2(\xi) = \sum_{i<j}(\xi_{ii}\xi_{jj} - \xi_{ij}\xi_{ji}).$$

We also showed in [9] that equality holds in (2.4) if and only if the matrix ξ is positive or negative definite and satisfies

$$\frac{\xi}{\mathbf{Tr}\xi} \geq \frac{H(k(x) + 2\frac{n-1}{n}\mu_2)}{nk_1 + 2(n-1)\mu_2} I. \tag{2.5}$$

Thus we obtain

$$W_{\min} \geq \inf_{<\theta(x)>=\theta} \inf_{u|_{\partial\Omega}=g} \fint_\Omega \left\{ \frac{A(\mathbf{div}\ u)^2}{\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2} - 4\mu_2 J_2\Big(e(u)\Big)\right\}dx, \tag{2.6}$$

where

$$A = (k_2 + 2\frac{n-1}{n}\mu_2)(k_1 + 2\frac{n-1}{n}\mu_2). \tag{2.7}$$

Equality holds in (2.6) if and only if $e(u)$ is positive or negative definite and satisfies (2.5) at every point x,

$$\frac{e(u)}{\mathbf{div}\, u} \geq \frac{1}{n} \cdot \frac{k_2 + 2\frac{n-1}{n}\mu_2}{\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2} I. \tag{2.8}$$

Now we are ready to derive an explicit optimal bound on $W_{\min}$ using the particular form of the relaxed problem (2.6).

3 Derivation of the bound.

Here we will derive an explicit bound on $W_{\min}$, keeping track of conditions that are necessary and sufficient for each inequality we use to become an equality. Our first step will use the following relations:

$$\begin{aligned} J_2\Big(e(u)\Big) &= J_2(\nabla u) - \tfrac{1}{8}|\nabla u - (\nabla u)^t|^2, \\ \fint_\Omega J_2(\nabla u)dx &= P(g), \end{aligned} \tag{3.1}$$

where $P(g)$ is a scalar functional that depends only on the boundary value $g(x)$. The first formula in (3.1) is a matter of elementary algebra; the second reflects the fact that $J_2(\nabla u)$ is a null-Lagrangian. We do not give the explicit formula for P because it is not essential to our result, but it can easily be derived using the divergence theorem. Combining (2.6) and (3.1) gives

$$W_{\min} \geq -4\mu_2 P(g) + \inf_{<\theta(x)>=\theta}\ \inf_{u|_{\partial\Omega}=g} \fint_\Omega \frac{A(\mathbf{div}\ u)^2}{\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2} dx. \tag{3.2}$$

Equality holds in (3.2) if and only if (2.8) holds, and in addition $\mathbf{curl}\ u = 0$.

The problem has simplified a lot now. On our second step we will establish an explicit bound on $W_{\min}$. It is an easy corollary of the Cauchy-Schwartz inequality that for any two functions $p \in L^2(\Omega)$ and $q > 0$

$$\Big(\fint_\Omega p(x)dx\Big)^2 \leq \Big(\fint_\Omega \frac{p^2(x)}{q(x)}dx\Big)\cdot\Big(\fint_\Omega q(x)dx\Big).$$

We apply this inequality to (3.2) by taking $p(x) = \mathbf{div}\ u$ and $q(x)$ equal to the denominator of (3.2). Thus we obtain the inequality:

$$\fint_\Omega \frac{(\mathbf{div}\ u)^2}{\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2} dx \geq \frac{\Big(\frac{1}{|\Omega|}\int_{\partial\Omega}(g\cdot n)ds\Big)^2}{\theta k_2 + (1-\theta)k_1 + 2\frac{n-1}{n}\mu_2}. \tag{3.3}$$

The inequality is achieved if and only if

$$\mathbf{div}\ u = \alpha\Big(\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2\Big), \tag{3.4}$$

where α is some constant. We can determine α easily by integrating (3.4) over Ω:

$$\alpha = \frac{\frac{1}{|\Omega|}\int_{\partial\Omega}(g\cdot n)ds}{\theta k_2 + (1-\theta)k_1 + 2\frac{n-1}{n}\mu_2}. \tag{3.5}$$

Finally, putting everything together we arrive at the explicit bound for $W_{\min}$:

$$W_{\min} \geq \frac{(k_2 + 2\frac{n-1}{n}\mu_2)(k_1 + 2\frac{n-1}{n}\mu_2)}{\theta k_2 + (1-\theta)k_1 + 2\frac{n-1}{n}\mu_2}\Big(\frac{1}{|\Omega|}\int_{\partial\Omega}(g\cdot n)ds\Big)^2 - 4\mu_2 P(g). \tag{3.6}$$

4 Optimality of the bound.

The inequality (3.6) represents a bound on $W_{\min}$ which is valid for any piecewise smooth bounded domain Ω in R^n and any displacement boundary condition g. However, this bound is not always optimal. The following theorem gives necessary and sufficient conditions for optimality of the bound (3.6).

Theorem 1 *The bound (3.6) is optimal if and only if there exists a convex function $\psi \in W^{2,\infty}(\Omega)$ with $\triangle\psi \le k_1 - k_2$ and*

$$\nabla\psi|_{\partial\Omega} = \frac{1}{\alpha}g(x) - \frac{1}{n}(k_2 + 2\frac{n-1}{n}\mu_2)x,$$

where α is given by (3.5).

Before we begin the proof, let us remark that in two space dimensions the question of existence of a function ψ satisfying the conditions of the theorem is equivalent to a problem of plastic limit analysis (see e.g. [6]). There the boundary traction g is considered "safe" if there exists a divergence-free field $\sigma(x)$ in Ω such that $\sigma \cdot \nu = g$ on $\partial\Omega$ and $\sigma(x) \in \Sigma$ for almost all $x \in \Omega$, where Σ is some closed convex set in the space of 2×2 symmetric matrices. The question is to determine which loads are safe and which are not. Using the Airy stress potential representation of a divergence-free field in two space dimensions we easily reduce the question of existence of ψ as in the theorem to a problem of plastic limit analysis. We now proceed with the proof of the theorem.

Proof. In the previous section we have determined that the inequality (3.6) becomes an equality if and only if there exist a displacement field u and a local volume fraction function $\theta(x)$ in Ω satisfying (2.8), (3.4) and **curl** $u = 0$. The last condition allows us to work with a scalar potential ϕ:

$$u = \nabla\phi. \tag{4.1}$$

We start by proving the necessity part of the theorem. So we assume that there are functions $\theta(x)$ and $\phi(x)$ satisfying (2.8), (3.4) and (4.1). In terms of the scalar potential ϕ (3.4) becomes

$$\triangle\phi = \alpha\Big(\theta(x)k_2 + (1-\theta(x))k_1 + 2\frac{n-1}{n}\mu_2\Big),$$

where α is given by (3.5). Substituting this equality in (2.8) we get

$$\frac{1}{\alpha}\nabla\nabla\phi \ge \frac{1}{n}(k_2 + 2\frac{n-1}{n}\mu_2)I.$$

We remark that if α were equal to 0 the Hessian $\nabla\nabla\phi$ would have to vanish at each point $x \in \Omega$, and u would have to be constant. Let us make a simple change of variables by considering

$$\psi(x) = \frac{1}{\alpha}\phi(x) - \frac{1}{2n}(k_2 + 2\frac{n-1}{n}\mu_2)|x|^2. \tag{4.2}$$

Then we obtain the following system of optimality conditions:

$$\begin{cases} \nabla\nabla\psi \geq 0, \\ \triangle\psi = (1-\theta(x))(k_1 - k_2), \\ \nabla\psi|_{\partial\Omega} = f, \end{cases} \tag{4.3}$$

where the boundary value f is given by

$$f(x) = \frac{1}{\alpha}g(x) - \frac{1}{n}(k_2 + 2\frac{n-1}{n}\mu_2)x. \tag{4.4}$$

Now the necessity in the theorem follows easily from (4.3).

To prove the sufficiency we will show how to construct the fields u and $\theta(x)$ that satisfy the optimality conditions (2.8), (3.4) and **curl** $u = 0$. We start with a convex function ψ satisfying the conditions of the theorem. Then the local volume fraction function $\theta(x)$ is given by

$$1 - \theta(x) = \frac{\triangle\psi}{k_1 - k_2} \tag{4.5}$$

and the local displacement field by

$$u(x) = \alpha\nabla\psi + \frac{\alpha}{n}(k_2 + 2\frac{n-1}{n}\mu_2)x. \tag{4.6}$$

Now it is very easy to see that (2.8) and (3.4) are satisfied. To obtain a design that achieves the bound (3.6) we should place an extremal microstructure corresponding to $\theta(x)$ and $e(x)$ at every point $x \in \Omega$. The design will be classical if the local volume fraction given by (4.5) takes only the values 0 and 1. The sufficiency is established. $\square$

We would like to remark that the optimal design is far from unique. At every point there is a whole menagerie of optimal microstructures to choose from: rank-2 laminates [1], [8], the confocal ellipse construction [10] and the Vigdergauz construction [11], to name just a few. In addition the function ψ is not unique in most cases.

We conclude the article by proving a simple necessary condition for (4.3) to be satisfied.

Notice that the first inequality in (4.3) implies that ψ is convex in Ω. But it is obvious that not all boundary values f can arise as the trace of the gradient of a convex function. The following proposition characterizes the set of functions f for which there is a convex ψ with $\nabla\psi|_{\partial\Omega} = f$.

Proposition 1 *Let $\Omega \subset R^n$ be open bounded and convex. Let $f : \partial\Omega \to R^n$ be a continuous trace of a gradient, i.e. $f|_{\partial\Omega} = \nabla F|_{\partial\Omega}$ for some C^1 function F. There exists a convex function ψ defined on Ω with $\nabla\psi|_{\partial\Omega} = f$ if and only if for all $\{x, y\} \subset \partial\Omega$*

$$\Big(f(y), x - y\Big) \leq F(x) - F(y), \tag{4.7}$$

with $f(x) = f(y)$ in case of equality.

Proof. First let us remark that the restriction of the function F to $\partial\Omega$ is defined uniquely up to an additive constant by f. Therefore (4.7) is a well-defined condition. The second remark is that the "only if" part is trivial. The inequality (4.7) follows from the geometric fact that a tangent plane to the graph of a convex function over a convex domain always lies below the graph. If there is equality in (4.7) it means that the tangent plane at y intersects the graph of ψ at x. By convexity, such a plane has to be tangent at x too, which implies that $f(x) = f(y)$.

Now suppose (4.7) is satisfied. Let

$$\psi(x) = \sup_{y\in\partial\Omega} \Big\{ F(y) + (f(y), x - y) \Big\}, \qquad x \in \overline{\Omega}. \tag{4.8}$$

Then $\psi(x)$ is convex, being a supremum of linear functions, and it is Lipschitz continuous on $\overline{\Omega}$. Our objective is to prove that $\nabla\psi$ exists and is equal to f on $\partial\Omega$. This is easily accomplished by means of a theorem from the non-smooth analysis ([4], Theorem 2.8.2 Corollary 2). According to this theorem the subgradient of ψ at $x \in \partial\Omega$ is the convex hull of $f(y)$ for all extremal y's. But condition (4.7) implies that for each $x \in \partial\Omega$ the value of all extremal $f(y)$ is uniquely defined by x and equal to $f(x)$. Thus the subgradient of ψ is in fact a gradient and $\nabla\psi(x) = f(x)$ for all $x \in \partial\Omega$.□

Obviously the function ψ we have constructed in the Proposition 1 does not satisfy the optimality conditions (4.3) because in general ψ is only Lipschitz continuous and not twice differentiable (by twice differentiable function we mean a function in $W^{2,\infty}$). At present, we do not know how prove the existence of a twice differentiable ψ. We conjecture that the necessary condition (4.7) is also a sufficient one, given some additional smoothness of f.

An even more serious problem arises in connection with the second condition in (4.3). It is obvious that we need further restrictions on the boundary value f in order to satisfy

$$\sup_{x\in\Omega} \triangle\psi \leq k_1 - k_2. \tag{4.9}$$

In fact, it is easy to verify that any function f arising in our problem through (4.4) must satisfy

$$\frac{1}{|\Omega|} \int_{\partial\Omega} (f \cdot n) ds = (1 - \theta)(k_1 - k_2) \tag{4.10}$$

As for sufficient conditions on f, this problem seems very hard and may not have a simple answer. But in the one dimensional case we can solve it geometrically (see the Appendix). This 1-D problem can provide some further necessary conditions on f by applying it to each pair of points $\{x, y\} \subset \partial\Omega$. It seems, however, that in this problem a truly multidimensional argument is called for.

5 Appendix: A one dimensional model problem.

Even for $n = 1$ the problem (4.3) is nontrivial. Here we solve the problem in this one dimensional case.

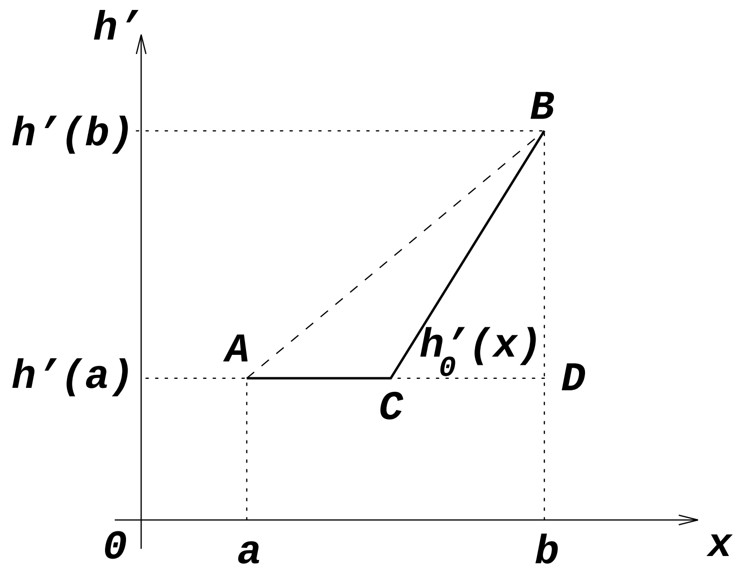

Figure 1: The geometric solution of the 1-D problem.

Suppose that we have boundary data for the function $\phi \in W^{2,\infty}([a,b])$ with $\phi'(b) > \phi'(a)$. We seek necessary and sufficient conditions on the four numbers $\phi(a)$, $\phi(b)$, $\phi'(a)$, $\phi'(b)$ for the existence of a convex function ψ satisfying

$$\psi(x) = \frac{1}{\alpha}\phi(x) - \frac{1}{2}k_2 x^2, \tag{5.1}$$

where

$$\alpha = \frac{\phi'(b) - \phi'(a)}{(b-a)(k_1(1-\theta) + k_2\theta)},$$

and

$$\psi''(x) \le k_1 - k_2. \tag{5.2}$$

The following proposition provides the tool for solving this problem.

Proposition 2 *Let A be the subset of $W^{2,\infty}([a,b])$ consisting of all functions h which are convex, with specified values for $h(a)$, $h(b)$, $h'(a)$, $h'(b)$. Then*

$$\inf_{h\in A} \|h''\|_\infty = \frac{1}{2}\max\left\{\frac{\Big(h'(b)-h'(a)\Big)^2}{(b-a)h'(b)+h(a)-h(b)}; \frac{\Big(h'(b)-h'(a)\Big)^2}{h(b)-h(a)-(b-a)h'(a)}\right\}. \tag{5.3}$$

Moreover, the extremal h always exists and is unique.

Proof. The formula (5.3) has a simple geometric interpretation in the plane (x, h'). If $h_0(x)$ is the optimal choice, then the graph of $h_0'(x)$ must join the two points $(a, h'(a))$

and $(b, h'(b))$ by a nondecreasing absolutely continuous curve with a given area under it (as $\int_a^b h'(x)dx = h(b) - h(a)$), and such that the maximum slope of the curve is as small as possible. Figure 1 shows the solution of the problem if the value of the area under the curve is less than the area of the trapezoid formed by x-axis, two vertical lines $x = a$ and $x = b$ and a dashed line AB.

To see that h_0 is the right choice, we observe that it is impossible to join any point in the triangle BCD with B while keeping the maximum slope no greater than that of BC. Also, any nondecreasing curve lying above ACB will have area under its graph larger than the area under ACB. Thus any nondecreasing function joining the points A and B has maximum slope at least that of BC, provided the area under its graph is equal to the area under ACB. Moreover, our argument clearly shows that a function attaining the infimum in (5.3) must coincide with $h_0(x)$. Calculating the maximal slope of $h_0'(x)$ we obtain the result of the proposition.□

According to (5.2) (cf. (4.9)) we need $\|\psi''\|_\infty \leq k_1 - k_2$. Applying the Proposition 2 and (5.1) we find, after a simple but lengthy calculation, that this holds if and only if the boundary data for the original function ϕ satisfy:

$$\frac{1}{2}\frac{k_1(1-\theta)^2 + k_2(1-(1-\theta)^2)}{k_1(1-\theta) + k_2\theta} \leq \frac{\phi(b) - \phi(a) - \phi'(a)(b-a)}{(\phi'(b) - \phi'(a))(b-a)} \leq \frac{1}{2}\frac{k_1(1-\theta^2) + k_2\theta^2}{k_1(1-\theta) + k_2\theta}.$$

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