The G-closure of two well-ordered, anisotropic conductors.

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Abstract

We give a complete solution to the G-closure problem for mixtures of two well ordered possibly anisotropic conductors. Both the G-closure with fixed volume fractions and the full G-closure are computed. The conductivity tensors are considered in a fixed frame and no rotations are allowed.

1 Introduction

The problem of describing all possible composites obtainable by mixing more than one material has been studied for many years and by many authors. The homogeneous composite material is in general anisotropic, and is characterized by its tensor of effective parameters. The set of all such tensors is called the G-closure, and the problem of describing this set is called the G-closure problem. Depending on the number, quantity and nature of the materials to be mixed we obtain different G-closure problems. This article solves one of them.

The G-closure problem was first addressed by Murat and Tartar [9] and independently by Lurie and Cherkaev [4], [5] generalizing the pioneering works of Hashin and Shtrikman [2]. The papers [4], [5], [9] completely solved the G-closure problem for two isotropic components using the method of compensated compactness (later renamed the translation method by Milton [6]). This article follows the approach of Kohn and Milton in [3] adapted to the case of anisotropic component materials.

Our main result is that the G-closure of two conductors with conductivity tensors A and B ($A < B$) mixed in fixed volume fractions θ_A, θ_B ($\theta_A+\theta_B=1$) consists of all tensors C^* satisfying the "trace bounds" (6) and the "Wiener bounds " (5) (see Theorem 3). Both of these bounds are well-known. The former bounds first appeared in their present form in [7], formulas (5.18),(5.20). The later were first derived by Wiener in 1912 [10]. By showing that these bounds characterize the G-closure, we are demonstrating that no better bounds are possible.

We also derive an expression for the full G-closure , i.e. the set of all composite conductivities obtainable when the volume fractions are not restricted (see (18)).

This paper is exclusively concerned with the case of two well-ordered conductivity tensors ($A < B$), not necessarily simultaneously diagonal. Analogous results have recently been obtained by Nesi, when A and B are simultaneously diagonal but not well-ordered [8].

2 Composite materials and the trace bounds

The goal of this section is a self-contained treatment of the trace bounds. We first describe the precise mathematical setting we will be dealing with. We consider two conductors with conductivities A and B — symmetric positive definite $n \times n$ matrices with $A < B$ in the sense of quadratic forms. There is no other restriction on A and B. Consider a composite made of these two conductors mixed in volume fractions θ_A, θ_B ($0 < \theta_A < 1$, $\theta_B = 1 - \theta_B$). By a composite we mean a conducting material with conductivity at point x

$$C(x) = A\chi_A(x) + B\chi_B(x); \tag{1}$$

here $\chi_A(x)$ and $\chi_B(x)$ are the indicator functions of the sets occupied by materials A and B respectively, with

$$\chi_A(x) + \chi_B(x) = 1.$$

Notice in formula (1) that we don't allow any rotation of the materials. Suppose our composite has fine scale structure. Mathematically this means that $C(x)$ is a rapidly oscillating function varying on a length scale ε. Then we will write $C(x/\varepsilon)$ instead of $C(x)$, where $C(y)$ is now a function varying on a length scale of order 1. It is sufficient to consider only the periodic composites, i.e. composites for which $C(y)$ is periodic with period cell Q, by results from the theory of G-convergence. For each ε we have the elliptic equation of electrostatics for the potential $u^{\varepsilon}(x)$ in the open bounded domain $\Omega \subset R^n$ occupied by the composite:

$$\nabla \cdot (C(x/\varepsilon)\nabla u^{\varepsilon}(x)) + f(x) = 0$$

$$u^{\varepsilon}|_{\partial\Omega} = 0,$$

where f is a suitable function ($f \in L^2(\Omega)$ will do). We want to study the behavior of its unique solution $u^{\varepsilon}(x)$ as $\varepsilon \to 0$. It can be proved [1] that $u^{\varepsilon}(x) \rightharpoonup u_0(x)$ in $H^1(\Omega)$ where u_0 satisfies the homogenized equation:

$$\nabla \cdot (C^* \nabla u_0(x)) + f(x) = 0$$

$$u_0|_{\partial\Omega} = 0$$

where C^* is a constant symmetric tensor called the effective conductivity tensor. Moreover C^* can be characterized as follows:

$$(C^*\xi, \xi) = \inf_{\phi} \fint_Q (C(y)(\xi + \nabla\phi), \xi + \nabla\phi) dy \tag{2}$$

where $(\cdot,\cdot)$ denotes the scalar product in R^n; $⨍_Q$ means $\frac{1}{\mathrm{Vol}(Q)}\int_Q$ and the inf is taken over all Q-periodic $H^1(Q)$ functions ϕ with mean value zero. Notice that C^* in fact does not depend neither on the function f nor on the region Ω. Formulas (1) and (2) are all we will need to study the effective conductivity of the composites. For a more detailed treatment see [1].

Our goal is to describe the set of all possible tensors C^* which can be obtained by varying the *microstructure*, that is, by varying the choice of $\chi_A(x)$ in (1). The idea is to prove some bounds on C^* then to show those bounds are optimal in the sense that any tensor satisfying the bounds arises as a C^* for some microstructure. In order to establish the bounds we use the variational formula (2) for C^*. Substituting ϕ =const in (2) we get an upper bound for C^*:

$$C^* \leq M$$

where

$$M = A\theta_A + B\theta_B \tag{3}$$

is the arithmetic mean. Similarly from the dual variational principle we get

$$C^* \geq H$$

where

$$H = (A^{-1}\theta_A + B^{-1}\theta_B)^{-1} \tag{4}$$

is the harmonic mean. The bounds

$$H \leq C^* \leq M \tag{5}$$

are called the Wiener bounds. They are very simple but unfortunately they are not optimal. We therefore need the "trace bounds":

Theorem 1 *The effective conductivity C^* satisfies*

$$\left.\begin{array}{l} \mathbf{Tr}(A(C^*-A)^{-1}) \leq \dfrac{1}{\theta_B}\mathbf{Tr}(A(B-A)^{-1}) + \dfrac{\theta_A}{\theta_B} \\ \mathbf{Tr}(B(B-C^*)^{-1}) \leq \dfrac{1}{\theta_A}\mathbf{Tr}(B(B-A)^{-1}) - \dfrac{\theta_B}{\theta_A} \end{array}\right\} \tag{6}$$

Proof. We begin by adding and subtracting $(\gamma(\xi+\nabla\phi), \xi+\nabla\phi)$ — the energy of a "reference medium" with constant conductivity tensor γ — on the right of (2):

$$(C^*\xi,\xi) = \inf_\phi ⨍_Q [((C(x)-\gamma)(\xi+\nabla\phi), \xi+\nabla\phi) + (\gamma(\xi+\nabla\phi), \xi+\nabla\phi)]dx \tag{7}$$

Here γ must be a positive definite symmetric matrix. It should satisfy $\gamma < A$ if we seek a lower bound and $\gamma > B$ if we seek an upper bound. Now we follow the approach of Kohn-Milton in [3] for deriving bounds on effective conductivity. We will emphasize only the differences. We proceed exactly as in [3] to get the Hashin-Shtrikman variational principle for the anisotropic case. We obtain for the lower bound after the dualization of the first term on right hand side of (7)

$$((C^* - \gamma)\xi, \xi) = \sup_{\sigma} ⨍_Q [2(\sigma, \xi) - ((C(x) - \gamma)^{-1}\sigma, \sigma) - (\sigma, \Gamma_\gamma \sigma)]dx \tag{8}$$

with $0 < \gamma < A$. And for the upper bound

$$((C^* - \gamma)\xi, \xi) = \inf_{\sigma} ⨍_Q [2(\sigma, \xi) - ((C(x) - \gamma)^{-1}\sigma, \sigma) - (\sigma, \Gamma_\gamma \sigma)]dx \tag{9}$$

with $\gamma > B$. In both formulas the sup(inf) is taken over $L^2(Q)$ vector fields σ, and the operator $\Gamma_\gamma : L^2(Q, R^n) \to L^2(Q, R^n)$ is defined by

$$\Gamma_\gamma \sigma = -\nabla \phi \tag{10}$$

where ϕ is the unique (mean value zero) periodic solution of

$$\nabla \cdot \gamma \nabla \phi = -\nabla \cdot \sigma \tag{11}$$

Notice that if γ, A and B are all scalar then (8) and (9) coincide with formulas (3.14) and (3.16) of [3] respectively. Then making a customary substitution $\sigma = \eta\chi_B$ for lower bound ($\sigma = \eta\chi_A$ for upper bound) and then optimizing explicitly in ξ we obtain bounds on C^*:

$$\theta_B{}^2(C^* - \gamma)^{-1} \leq \theta_B(B - \gamma)^{-1} + F_\gamma^B$$

$$\theta_A{}^2(C^* - \gamma)^{-1} \geq \theta_A(A - \gamma)^{-1} + F_\gamma^A$$

where F_γ^A is the matrix of "geometric parameters" defined by

$$(F_\gamma^A \eta, \eta) = ⨍_Q (\eta\chi_A, \Gamma_\gamma(\eta\chi_A))dx \tag{12}$$

where $\eta \in R^n$. Again as in [3] we prove that

$$\mathbf{Tr}(\gamma F_\gamma^A) = \theta_A(1 - \theta_A) = \theta_A\theta_B$$

This is most easily seen in the case when Q is a unit cube, by using the Fourier series decomposition on Q. By Parseval's identity applied to (12), and using the definition of Γ_γ (10), (11), we obtain:

$$F_\gamma^A = \sum_{k \neq 0} \frac{k \otimes k}{(\gamma k, k)} |\widehat{\chi}_A(k)|^2,$$

where $\widehat{\chi}_A(k)$ are the Fourier coefficients of the function $\chi_A(x)$. The result then follows easily. Now using the fact that

$$T_1 \geq T_2 \Rightarrow \gamma^{1/2} T_1 \gamma^{1/2} \geq \gamma^{1/2} T_2 \gamma^{1/2} \Rightarrow \mathbf{Tr}(\gamma T_1) \geq \mathbf{Tr}(\gamma T_2)$$

for any two matrices T_1 and T_2, we get the general trace bounds for anisotropic case:

$$\mathbf{Tr}(\gamma(C^* - \gamma)^{-1}) \leq \frac{1}{\theta_B}\mathbf{Tr}(\gamma(B - \gamma)^{-1}) + \frac{\theta_A}{\theta_B}$$

$$\mathbf{Tr}(\gamma(\gamma - C^*)^{-1}) \leq \frac{1}{\theta_A}\mathbf{Tr}(\gamma(\gamma - A)^{-1}) - \frac{\theta_B}{\theta_A}$$

Letting $\gamma \uparrow A$ in the first inequality and $\gamma \downarrow B$ in the second one we get the optimal trace bounds (6).

Q. E. D.

The above argument is valid only for the case $A \leq B$. In the non-well-ordered case one should use more powerful translation method (for treatment see [8]).

In (6) the first inequality represents a lower bound on C^* while the second one represents an upper bound. It is convenient for later use to rewrite these bounds in a different way:

$$\left.\begin{aligned} \mathbf{Tr}(A(C^* - A)^{-1}) &\leq \mathbf{Tr}(A(M - A)^{-1}) + \frac{\theta_A}{\theta_B} \\ \mathbf{Tr}(B(B - C^*)^{-1}) &\leq \mathbf{Tr}(B(B - M)^{-1}) - \frac{\theta_B}{\theta_A} \end{aligned}\right\} \tag{13}$$

This is equivalent to (6) because one can check that

$$\theta_B(B - A) = M - A.$$

We now turn to the attainability of the trace bounds. In what follows we assume that the period cell Q is a unit cube in R^n. Any other case is easily reduced to this one by a similarity transform. The statement below and its proof are due to L. Tartar [9]. We repeat Tartar's argument for the sake of completeness.

Theorem 2 *If a symmetric matrix C with $A < C \leq M$ achieves equality in one of the bounds (6) then it is attainable by some composite.*

Proof. The idea of the proof is to describe a class of microstructures whose conductivities are easy to compute explicitly and rich enough to achieve any matrix satisfying the conditions of the theorem. Such a class is the family of laminates. We start with the rank-1 lamination formula. Consider a composite where materials A and B are arranged in layers orthogonal to a vector e_1 . In this case C^* satisfies the relations ([9], Proposition 3):

$$\left.\begin{aligned} \theta_B(C^* - A)^{-1} &= (B - A)^{-1} + \theta_A \frac{e_1 \otimes e_1}{(Ae_1, e_1)} \\ \theta_A(C^* - B)^{-1} &= (A - B)^{-1} + \theta_B \frac{e_1 \otimes e_1}{(Be_1, e_1)} \end{aligned}\right\} \tag{14}$$

We may now layer this composite with the material A in layers orthogonal to e_2. Let us denote the relative volume fractions of material A in the whole composite used in each step as ρ_1 and ρ_2 respectively ($\rho_1 + \rho_2 = 1$) and let the volume fraction of A in the whole composite be θ_A. Then a brief calculation shows that C^* satisfies

$$\theta_B(C^* - A)^{-1} = (B - A)^{-1} + \theta_A \sum_{i=1}^{2} \rho_i \frac{e_i \otimes e_i}{(Ae_i, e_i)}.$$

If we repeat the process m times, each time layering the resulting composite with material A, then we obtain a composite with C^* satisfying ([9], Proposition 4)

$$\theta_B(C^* - A)^{-1} = (B - A)^{-1} + \theta_A \sum_{i=1}^{m} \rho_i \frac{e_i \otimes e_i}{(Ae_i, e_i)}, \tag{15}$$

where $\rho_i \in [0, 1]$ and $\sum_{i=1}^{m} \rho_i = 1$. It is easy to show that varying the volume fractions ρ_i at each step but keeping θ_A fixed we can get composites satisfying (15) with an arbitrary admissible set $\{\rho_i\}$ and arbitrary vectors $\{e_i\}$. Notice that for $m = n$ the matrix

$$T = \sum_{i=1}^{n} \rho_i \frac{e_i \otimes e_i}{(Ae_i, e_i)}$$

can be any symmetric positive semidefinite matrix with the property

$$\mathbf{Tr}(AT) = 1.$$

In fact if

$$A^{1/2}TA^{1/2} = \sum_{i=1}^{n} \mu_i (v_i \otimes v_i)$$

is orthonormal eigendecomposition of $A^{1/2}TA^{1/2}$ then we may set

$$\rho_i = \mu_i$$

and take e_i such that

$$\frac{A^{1/2}e_i}{\| A^{1/2}e_i \|} = v_i$$

Now let C satisfy conditions of the theorem. Consider the matrix

$$T = \frac{\theta_B}{\theta_A}(C - A)^{-1} - \frac{1}{\theta_A}(B - A)^{-1}$$

Notice that since $C > A$, the condition $T \geq 0$ is equivalent to the condition $C \leq M$. Also the condition that C achieves equality in the lower bound (6) is exactly the condition

$$\mathbf{Tr}(AT) = 1.$$

Therefore there exists a laminate (of rank n, in general) with effective conductivity C^* such that

$$\theta_B(C^* - A)^{-1} - (B - A)^{-1} = \theta_B(C - A)^{-1} - (B - A)^{-1},$$

which yields $C = C^*$. The attainability of the lower bound is proved. The upper bound is treated similarly.

Q. E. D.

Let $\tilde{G}$ be the set of all symmetric second order tensors described by the above bounds , and let G represent the G-closure of $(A, B, \theta_A, \theta_B)$. Our task is to show that $\tilde{G} = G$.

3 Attainability of $\tilde{G}$.

In this section we prove the main result of the paper: $G = \tilde{G}$. But first we need some simple algebraic properties of the trace bounds with respect to rank-1 perturbations. We start with some technical lemmas from linear algebra. Let A and B be symmetric $n \times n$ matrices with $A < B$ in the sense of quadratic forms. Let

$$X = X(\lambda, e) = A + \lambda e \otimes e, \qquad \lambda > 0.$$

When λ is small then $X < B$. As λ increases X also increases and at some moment $B - X(\lambda, e)$ ceases to be positive definite.

Lemma 1 *The first value of λ when $B - X$ ceases to be positive definite is*

$$\lambda(e) = \frac{1}{((B-A)^{-1}e, e)}$$

Proof. When $\lambda = \lambda(e), \exists y \in R^n \setminus \{0\}$ such that $((B - X)y, y) = 0$ but $B - X$ is still positive semidefinite. Therefore $Xy = By$ or

$$\lambda(e)(e, y)e = (B - A)y$$

$$y = \lambda(e)(e, y)(B - A)^{-1}e$$

The last relation implies that $(e, y) \neq 0$ since $y \neq 0$. Taking the inner product with e gives

$$(e, y) = \lambda(e)(e, y)((B - A)^{-1}e, e).$$

Since $(e, y) \neq 0$ we get

$$\lambda(e) = \frac{1}{((B-A)^{-1}e, e)}.$$

Lemma 2 *Let $A < C < B$. Then $\mathbf{Tr}(A(C + \lambda e \otimes e - A)^{-1})$ is a decreasing function and $\mathbf{Tr}(B(B - C - \lambda e \otimes e)^{-1})$ is an increasing function of λ on the intervals of continuity.*

Proof. From the well-known formula

$$(C + \lambda e \otimes e)^{-1} = C^{-1} - \frac{\lambda}{1 + \lambda(C^{-1}e, e)} C^{-1}e \otimes C^{-1}e$$

we obtain

$$\mathbf{Tr}(A(C + \lambda e \otimes e - A)^{-1}) = \mathbf{Tr}(A(C - A)^{-1}) - \lambda \frac{((C-A)^{-1}A(C-A)^{-1}e, e)}{1 + \lambda((C-A)^{-1}e, e)} \tag{16}$$

$$\mathbf{Tr}(B(B - C - \lambda e \otimes e)^{-1}) = \mathbf{Tr}(B(B - C)^{-1}) + \lambda \frac{((B-C)^{-1}B(B-C)^{-1}e, e)}{1 - \lambda((B-C)^{-1}e, e)} \tag{17}$$

from which the result follows easily. Note that if λ is such that $A < C + \lambda e \otimes e < B$ then from Lemma 1 we conclude that $\lambda \in (\lambda', \lambda'')$ where

$$\lambda' = -\frac{1}{((C-A)^{-1}e, e)}, \qquad \lambda'' = \frac{1}{((B-C)^{-1}e, e)}$$

and therefore both functions are continuous and monotone there.

Now we are ready to prove the main result of the article.

Theorem 3 *Every matrix C in the set $\tilde{G}$ (defined by the inequalities (5), (6)) is attainable as a composite mixture of conductors A and B in the volume fractions θ_A, θ_B.*

Proof. The proof is by induction in r =rank$(M-C)$. Case $r=0$ (i.e. $C=M$) can not occur as is vividly seen from (13). Let's prove the statement for $r=1$. Suppose $C_0 \in \tilde{G}$ and

$$C_0 = M - \lambda_0 e \otimes e, \quad \lambda_0 > 0$$

Let

$$Y = Y(\lambda) = M - \lambda e \otimes e.$$

As λ decreases from λ_0 to 0 then by monotonicity (Lemma 2) there exists $\lambda_1 \in (0, \lambda_0]$ such that

$$C_1 = Y(\lambda_1) = M - \lambda_1 e \otimes e$$

achieves equality in the upper trace bound. (We use here the fact that $Y(0) = M$ does not satisfy the trace bounds.) Since $C_0 \in \tilde{G}$ and $C_1 \geq C_0$ it is clear that C_1 satisfies all the conditions of Theorem 2. Therefore C_1 is attained, say by a composite q_1. Now let λ increase from λ_0 to $\lambda^* = 1/((M-A)^{-1}e, e)$. (Notice that $\lambda^* > \lambda_0$. In fact

$$Y(\lambda_0) = C_0 \in \tilde{G} \Rightarrow Y(\lambda_0) > H > A,$$

whereas by Lemma 1, $Y(\lambda^*) - A$ is singular). From (16) we see that

$$\mathbf{Tr}(A(Y(\lambda) - A)^{-1}) \to +\infty \mathrm{as} \lambda \uparrow \lambda^*.$$

So, by monotonicity (Lemma 2) $\exists \lambda_2 \in [\lambda_0, \lambda^*)$ such that

$$C_2 = Y(\lambda_2) = M - \lambda_2 e \otimes e$$

achieves equality in the lower trace bound. It is easy to see that C_2 satisfies all the conditions of the Theorem 2; so it is attained, say by a composite q_2. If we now layer composites q_1 and q_2 with layers orthogonal to e adjusting appropriately the relative volume fractions of q_1 and q_2, we can obtain a composite with conductivity tensor exactly equal to C_0 (this is most easily seen from formulas (14)). Thus the statement is proved for $r=1$. (After a more subtle analysis it can be shown that $\lambda_1 = \lambda_2 = \lambda_0$, but this is not essential here.)

Now assume that the statement is proved for $r = 1, 2, 3, \ldots, k$. Let's prove it for $r = k+1$. Again, we suppose $C_0 \in \tilde{G}$ with r =rank$(M - C_0) = k+1$. Since $r > 1, \exists e \neq 0$ such that $(Me, e) > (C_0 e, e), \quad e \in L^{\perp}$ with $L = \{\xi : M\xi = C_0 \xi\}$. Consider

$$Z = Z(\lambda) = C_0 + \lambda e \otimes e.$$

As λ increases from 0 there could be two possibilities: either $\text{rank}(M - Z)$ becomes less than $k + 1$ while Z still satisfies trace bounds or, else Z will achieve equality in the upper trace bound. (By Lemma 2 the lower trace bound and the condition $Z > A$ will always be satisfied.) In the latter case by Theorem 2 and in the former case by the induction hypothesis, there exists $\lambda_1 \geq 0$ such that

$$C_1 = Z(\lambda_1) = C_0 + \lambda_1 e \otimes e$$

is attainable by composite w_1. Now as λ decreases from 0 then $\text{rank}(M - Z)$ can not change and by Lemma 2 the upper trace bound and condition $Z < B$ will always be satisfied. So we may proceed exactly as for $r = 1$, except that now λ varies on the interval $[0, \bar{\lambda})$ where

$$\bar{\lambda} = \frac{1}{((C_0 - A)^{-1} e, e)}.$$

As before we obtain a matrix

$$C_2 = Z(\lambda_2) = C_0 - \lambda_2 e \otimes e, \quad \lambda_2 \in [0, \bar{\lambda})$$

which satisfies the conditions of Theorem 2 and therefore is attained by a composite w_2. Then we layer w_1 and w_2 together to obtain C_0. This completes the induction. So, we have proved that $G = \tilde{G}$.

Q. E. D.

We remark that the set $G = \tilde{G}$ is convex because the functions $\mathbf{Tr}(B(B - C)^{-1})$ and $\mathbf{Tr}(A(C - A)^{-1})$ are convex in C. This is easily established using the matrix version of inequality between harmonic mean and arithmetic mean, which can be proved by the method of simultaneous diagonalization.

What we have described here is the G-closure of two materials mixed in fixed volume fractions. This enables us to describe the full G-closure, i.e. the set of all possible effective tensors one can get mixing two given materials. Obviously it is the union of all sets G described above when θ_A ranges from 0 to 1. To describe the set analytically we can view trace bounds in the form (6) as bounds on two independent numbers $\mathbf{Tr}(B(B - C^*)^{-1})$ and $\mathbf{Tr}(A(C^* - A)^{-1})$. We need then take into account only the upper of the Wiener bounds and the condition $C^* \geq A$ by virtue of Theorem 2. It is then quite easy to show that the full G-closure is described as follows:

$$\left.\begin{array}{l} B \geq C^* \geq A \\ \mathbf{Tr}(B(B - C^*)^{-1})\mathbf{Tr}(A(C^* - A)^{-1}) \leq \mathbf{Tr}(A(B - A)^{-1})\mathbf{Tr}(B(B - C^*)^{-1}) + \\ \mathbf{Tr}(B(B - A)^{-1})\mathbf{Tr}(A(C^* - A)^{-1}) + n - 1 \\ (C^* - A)\mathbf{Tr}(A(C^* - A)^{-1}) + C^* - B \leq (B - A)\mathbf{Tr}(A(B - A)^{-1}) \end{array}\right\} \tag{18}$$

Indeed, if C^* satisfies these relations then $C^* \in G(\theta_0, A, B)$, where

$$\theta_0 = \frac{\mathbf{Tr}(A(C^* - A)^{-1}) - \mathbf{Tr}(A(B - A)^{-1})}{1 + \mathbf{Tr}(A(C^* - A)^{-1})}.$$

Conversely if $C^* \in G(\theta_A, A, B)$ for some θ_A then one can check that $\theta_0 \leq \theta_A$ and thus the above inequalities hold. In 2-D and for isotropic materials the above formulas give the familiar picture of the full G-closure.

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