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A NOTE ON THE BULK MODULUS OF A BINARY ELASTIC MIXTURE

M. K. KOLEV and K. Z. MARKOV

The Hashin-Shtrikman and Walpole bounds on the effective bulk modulus of a binary elastic mixture are revisited. A simple method of derivation is given as a generalization of the approach, recently proposed by one of the authors in the absorption and scalar conductivity problems for a two-phase medium.

Keywords: two-phase random media, effective bulk modulus, variational estimates, Hashin-Shtrikman and Walpole bounds

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The aim of this note is to present and discuss a simple derivation of the well-known two-point estimates on the effective bulk modulus of a binary elastic mixture, due to Hashin and Shtrikman [1] and Walpole [2]. The basic idea is a straightforward generalization of the approach, used by one of the authors in the absorption and scalar conductivity cases [3].

Assume that the mixture is statistically homogeneous and isotropic. Let

$$\chi_i(x) = \begin{cases} 1, & \text{if } x \in \Omega_i, \\ 0, & \text{otherwise,} \end{cases} \quad (1)$$

be the characteristic function of the region Ω_i , occupied by one of the constituents, labelled 'i', $i = 1, 2$, so that $\chi_1(x) + \chi_2(x) = 1$. Hereafter, all quantities, pertaining to the region Ω_1 or Ω_2 , are supplied with the subscript '1' or '2', respectively.

The statistical properties of the medium follow from the set of multipoint moments of one of the functions $\chi_i(x)$, say $\chi_2(x)$, for definiteness, or, which is the

same, by the volume fraction $\eta_2 = \langle \chi_2(x) \rangle$ of the phase ‘2’, and the multipoint moments

$$M_2(x) = \langle \chi_2'(0)\chi_2'(x) \rangle, \quad M_3(x, y) = \langle \chi_2'(0)\chi_2'(x_1)\chi_2'(y) \rangle, \dots, \quad (2)$$

with $\chi_2'(x) = \chi_2(x) - \eta_2$ being the fluctuating part of the field $\chi_2(x)$, see, e.g. [4]. The angled brackets $\langle \cdot \rangle$ hereafter denote ensemble averaging. One point could be taken at the origin, because of the assumed statistical homogeneity, as already done in (2).

Assuming also the constituents isotropic, the fourth-rank tensor of elastic moduli of the medium, $\mathbf{L}(x)$ is a random field of the familiar form

$$\begin{aligned} \mathbf{L}(x) &= 3k(x)\mathbf{J}' + 2\mu(x)\mathbf{J}'', \\ k(x) &= k_1\chi_1(x) + k_2\chi_2(x) = \langle k \rangle + [k]\chi_2'(x), \\ \mu(x) &= \mu_1\chi_1(x) + \mu_2\chi_2(x) = \langle \mu \rangle + [\mu]\chi_2'(x), \end{aligned} \quad (3)$$

where k and μ stand, as usual, for the bulk and shear modulus, respectively. The square brackets denote the jumps of the appropriate quantities, say, $[k] = k_2 - k_1$, $[\mu] = \mu_2 - \mu_1$, etc. In Eq. (3), \mathbf{J}' and \mathbf{J}'' are the basic isotropic fourth-rank tensors with the Cartesian components

$$J'_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}, \quad J''_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right). \quad (4)$$

The displacement field $u(x)$ in the medium, at the absence of body forces, is governed by the well-known equations

$$\begin{aligned} \nabla \cdot \boldsymbol{\sigma}(x) &= 0, \\ \boldsymbol{\sigma}(x) &= \mathbf{L}(x) : \boldsymbol{\varepsilon}(x) = k(x)\theta(x)\mathbf{I} + 2\mu(x)\mathbf{d}(x), \\ \boldsymbol{\varepsilon} &= \frac{1}{2}(\nabla u + u\nabla), \quad \mathbf{d}(x) = \boldsymbol{\varepsilon}(x) - \frac{1}{3}\theta(x)\mathbf{I}, \end{aligned} \quad (5)$$

where $\boldsymbol{\sigma}$ denotes the stress tensor, $\boldsymbol{\varepsilon}$ is the small strain tensor, generated by the displacement field $u(x)$, \mathbf{d} is the strain deviator, and $\theta = \text{tr } \boldsymbol{\varepsilon}$ is the volumetric strain. The colon designates contraction with respect to two pairs of indices and \mathbf{I} is the unit second-rank tensor.

The system (5) is supplied with the condition

$$\langle \boldsymbol{\varepsilon}(x) \rangle = \mathbf{E}, \quad (6)$$

prescribing the macroscopic strain tensor \mathbf{E} , imposed upon the medium.

Recall [4] that the random problem (5), (6) is equivalent to the variational principle of classical type

$$\begin{aligned} W[\boldsymbol{\varepsilon}(x)] &= \langle \boldsymbol{\varepsilon}(x) : \mathbf{L}(x) : \boldsymbol{\varepsilon}(x) \rangle \rightarrow \min, \\ \min W &= \mathbf{E} : \mathbf{L}^* : \mathbf{E}. \end{aligned} \quad (7)$$

The energy functional W is considered over the class of random fields $u(x)$ that generate strain fields $\boldsymbol{\varepsilon}(x)$, complying with the condition (6). In Eq. (7), \mathbf{L}^* is the tensor of effective elastic moduli for the medium which, in the isotropic case under study, has the form

$$\mathbf{L}^* = 3k^* \mathbf{J}' + 2\mu^* \mathbf{J}'', \quad (8)$$

where k^* and μ^* are the effective bulk and shear modulus of the mixture, respectively.

Consider, guided by [3], the class of trial fields for the variational principle (7):

$$\mathcal{K}^{(1)} = \left\{ \tilde{u}(x) \mid \tilde{u}(x) = \mathbf{E} \cdot x - \alpha \int \nabla G(x-y) \chi_2'(y) d^3 y \right\}, \quad (9)$$

having assumed that \mathbf{E} is spherical

$$\mathbf{E} = \frac{1}{3} \mathbf{I}, \quad G(x) = \frac{1}{4\pi|x|}, \quad (10)$$

and α is an adjustable scalar parameter. Hereafter the integrals are over the whole \mathbb{R}^3 , if the integration domain is not explicitly indicated.

The energy functional W , when restricted over $\mathcal{K}^{(1)}$, becomes a quadratic function of α :

$$\begin{aligned} W[\tilde{u}(x)] &= A - 2B\alpha + C\alpha^2, \quad A = \langle k \rangle, \quad B = [k] M_2(0), \\ C &= \langle \lambda \rangle M_2(0) + [\lambda] M_3(0, 0) + 2 \langle \mu \rangle P_2 + 2[\mu] P_3, \end{aligned} \quad (11)$$

with the dimensionless statistical parameters for the medium, defined as follows:

$$\begin{aligned} P_2 &= \iint \nabla \nabla G(y_1) : \nabla \nabla G(y_2) M_2(y_1 - y_2) d^3 y_1 d^3 y_2, \\ P_3 &= \iint \nabla \nabla G(y_1) : \nabla \nabla G(y_2) M_3(y_1, y_2) d^3 y_1 d^3 y_2; \end{aligned} \quad (12)$$

$\lambda = k - \frac{2}{3}\mu$ is the familiar Lamé constant.

Note that for the isotropic binary medium under study

$$M_2(0) = \langle \chi_2'^2(0) \rangle = \eta_1 \eta_2, \quad M_3(0) = \langle \chi_2'^3(0) \rangle = \eta_1 \eta_2 (\eta_1 - \eta_2). \quad (13)$$

Moreover, the parameter P_2 can be easily evaluated, having integrated by parts and noting that $G(x)$ is the well-known Green function for the Laplacian:

$$P_2 = M_2(0) = \eta_1 \eta_2. \quad (14)$$

The variational principle (7), together with (11), implies

$$k^* \leq W[\tilde{u}(x)] = A - 2B\alpha + C\alpha^2, \quad \forall \alpha. \quad (15)$$

In particular, at $\alpha = 0$ one has

$$k^* \leq \langle k \rangle \quad (16)$$

which, obviously, is the elementary (Voigt) bound on k^* .

Next, optimizing (15) with respect to α , one gets another estimate on k^* :

$$k^* \leq A - \frac{B^2}{C}, \quad (17a)$$

i.e.

$$k^* \leq \langle k \rangle - \frac{\eta_1 \eta_2 [k]^2}{\langle \lambda + 2\mu \rangle + ([\lambda] + 2[\mu]I_3)(\eta_1 - \eta_2)}, \quad (17b)$$

where

$$I_3 = \frac{1}{\eta_1 \eta_2 (\eta_1 - \eta_2)} P_3 \quad (18)$$

is the statistical parameter that appears in the perturbation expansion of κ^* for a weakly inhomogeneous medium, see [5], and also in the Beran's bound on the effective conductivity constant [6]. A simple check shows that (18) coincides with the upper bound on k^* , due to Beran and Molyneux (BM) [7].

The main problem in specifying the bound (17b) is just the three-point parameter I_3 whose evaluation for special and realistic random constitution is non-trivial. Recall that in many cases it is more convenient to employ, instead of I_3 , the Torquato-Milton parameter ζ_1 , see [8, 9], defined as a certain integral, similar to P_3 (see, e.g. the Torquato review [10]). Without going into detail, we shall only point out the formula

$$3(\eta_2 - \eta_1)I_3 = 2\zeta_1 + 3\eta_1 - \eta_2. \quad (19)$$

The bound (18) should be at least as good as the elementary bound (16) (since the energy functional is minimized over a broader class of trial fields). This implies that

$$C > 0, \quad AC - B^2 \geq 0, \quad (20)$$

because $k^* \geq 0$. Since $A = \langle k \rangle > 0$, $C \geq B^2/A > 0$, which means that the second inequality in (20) is the stronger one. Using the expressions for A , B and C from (11), we can write the latter in the form

$$\langle \lambda + 2\mu \rangle + ([\lambda] + 2[\mu]I_3)(\eta_1 - \eta_2) - \frac{[k]^2}{\langle k \rangle} \eta_1 \eta_2 \geq 0. \quad (21)$$

The inequality (21) should hold for every "realistic" choice of the elastic moduli of the constituents (i.e. for which the appropriate elastic energy is positive-definite). This implies

$$\frac{1}{3}\eta_1 - \eta_2 \leq (\eta_1 - \eta_2)I_3 \leq \eta_1 - \frac{1}{3}\eta_2. \quad (22)$$

Note that (22) drastically simplifies, when the parameter ζ_1 is used, instead of I_3 , see (19). Namely, it states then that $0 \leq \zeta_1 \leq 1$, which is a well-known fact [8, 9].

However, keeping I_3 in the BM-bound (17b) has its advantages. Namely, by means of (22) we can exclude the product $(\eta_1 - \eta_2)I_3$ from this bound. Depending on the sign of $[\mu] = \mu_2 - \mu_1$, we should use to this end the upper or lower bound (22). The final result reads

$$\begin{aligned} k^* &\leq \langle k \rangle - \frac{\eta_1 \eta_2 [k]^2}{\lambda_1 + 2\mu_1 + \eta_1 [k]}, & \text{if } \mu_2 \leq \mu_1, \\ k^* &\leq \langle k \rangle - \frac{\eta_1 \eta_2 [k]^2}{\lambda_2 + 2\mu_2 - \eta_2 [k]}, & \text{if } \mu_2 \geq \mu_1. \end{aligned} \quad (23)$$

In the so-called “well-ordered” case, when $(k_2 - k_1)(\mu_2 - \mu_1) > 0$, the first of the estimates (23) coincides with the Hashin-Shtrikman (HS) bound on k^* , provided that not only $\mu_2 \leq \mu_1$, but also $k_2 \leq k_1$, see [1]. This unnecessary restriction was removed by Walpole [2]. It is easily seen that our bounds (23) are just the Walpole bounds in which no requirements are put on the sign of $k_2 - k_1$.

The derivation of the lower bound, corresponding to (23), is fully similar. In this case we write the elastic energy (7) by means of the stress tensor:

$$\begin{aligned} W[\boldsymbol{\sigma}(x)] &= \langle \boldsymbol{\sigma}(x) : \mathbf{L}^{-1}(x) : \boldsymbol{\sigma}(x) \rangle \rightarrow \min, \\ \min W &= \boldsymbol{\Sigma} : \mathbf{L}^{*-1} : \boldsymbol{\Sigma}. \end{aligned} \quad (24)$$

The functional W is considered now over the class of trial fields, such that

$$\nabla \cdot \boldsymbol{\sigma}(x) = 0, \quad \langle \boldsymbol{\sigma}(x) \rangle = \boldsymbol{\Sigma}, \quad (25)$$

with a prescribed macrostress tensor $\boldsymbol{\Sigma}$, imposed upon the medium.

The functional W in (24) is minimized now over the class of trial fields

$$\mathcal{N}^{(1)} = \left\{ \tilde{\boldsymbol{\sigma}}(x) \mid \tilde{\boldsymbol{\sigma}}(x) = \boldsymbol{\Sigma} + \alpha \left[\int \nabla \nabla G(x-y) \chi'_2(y) d^3y + \mathbf{I} \chi'_2(y) \right] \right\}, \quad (26)$$

with the spherical $\boldsymbol{\Sigma} = \frac{1}{3} \mathbf{I}$ and an adjustable scalar parameter α , $G(x)$ being the function defined in (10). The straightforward manipulations are omitted and the final result reads

$$\begin{aligned} k^* &\geq \langle k \rangle - \frac{\eta_1 \eta_2 [k]^2}{\lambda_2 + 2\mu_2 - \eta_2 [k]}, & \text{if } \mu_2 \leq \mu_1, \\ k^* &\geq \langle k \rangle - \frac{\eta_1 \eta_2 [k]^2}{\lambda_1 + 2\mu_1 + \eta_1 [k]}, & \text{if } \mu_2 \geq \mu_1. \end{aligned} \quad (27)$$

The inequalities (27), combined with (23), are just the Walpole bounds on the effective bulk modulus of a binary mixture, see [2] and also [11], which are a direct generalization of the Hashin-Shtrikman result with the condition of “well-orderness” removed. Here we have demonstrated how this classical estimate shows up simply and naturally within the frame of the general method, recently developed by one of the authors [3] in the absorption and scalar conductivity contexts.

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Mikhail K. KOLEV
 Faculty of Mathematics and
 Informatics, South-West University
 Blagoevgrad, Bulgaria
 E-mail: mkkolev@aix.swu.bg

Konstantin Z. MARKOV
 Faculty of Mathematics and Informatics
 “St. Kliment Ohridski” University of Sofia
 BG-1164 Sofia, Bulgaria
 E-mail: kmarkov@fmi.uni-sofia.bg