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A NOTE ON THE BULK MODULUS OF A BINARY ELASTIC MIXTURE

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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

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

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

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

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

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

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

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

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

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

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 $\theta = \operatorname{tr}\boldsymbol{\varepsilon}$ 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

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

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:

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

The energy functional W is considered over the class of random fields $u(x)$ that generate strain fields $\varepsilon(x)$, 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

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

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):

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

having assumed that $\mathbf{E}$ is spherical

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

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:

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

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

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

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

Note that for the isotropic binary medium under study

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

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:

$$P_2 = M_2(0) = \eta_1\eta_2. \tag{14}$$

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

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

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

$$k^* \leq \langle k \rangle \tag{16}$$

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

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

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

i.e.

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

where

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

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 nontrivial. 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

$$3(\eta_2 - \eta_1)I_3 = 2\zeta_1 + 3\eta_1 - \eta_2. \tag{19}$$

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

$$C > 0, \quad AC - B^2 \geq 0, \tag{20}$$

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

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

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

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

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

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

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:

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

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

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

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

$$\mathcal{N}^{(1)} = \left\{ \widetilde{\boldsymbol{\sigma}}(x) \mid \widetilde{\boldsymbol{\sigma}}(x) = \boldsymbol{\Sigma} + \alpha \left[\int \nabla\nabla G(x-y)\chi_2'(y)\, d^3y + \mathbf{I}\chi_2'(y) \right] \right\} \tag{26}$$

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

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

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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