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BOUNDS ON THE EFFECTIVE ABSORPTION COEFFICIENT OF RANDOM MEDIA

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ABSTRACT

Variational estimates (upper and lower) are derived for the effective absorption coefficient (sink strength) of a random medium. The estimates are three-point, i.e., they employ statistical information, contained in the ℓ-point correlation functions for the medium up to $\ell = 3$, and could be viewed as counterparts of the well-known Beran's bounds in the scalar conductivity problem. Explicit results are obtained for Miller's cellular media.

INTRODUCTION

Consider the steady-state equation

$$\Delta\varphi(\mathbf{x}) - k^2(\mathbf{x})\varphi(\mathbf{x}) + K = 0, \tag{1}$$

that governs, at the expense of some simplifying assumptions, the concentration $\varphi(\mathbf{x})$ of a diffusing species (say, irradiation defects), generated at the constant rate K, in a random absorbing (lossy) medium, see [1] for references and more details. The absorption coefficient $k^2(\mathbf{x})$ is a given random field, assumed positive and statistically homogeneous and isotropic. The problem is to evaluate the random field $\varphi(\mathbf{x})$, i.e., all its multipoint correlations, and, in particular, to find the mean defect concentration $\langle\varphi(\mathbf{x})\rangle$; the brackets $\langle\cdot\rangle$ hereafter denote ensemble averaging. The latter value allows to obtain the effective absorption coefficient (sink strength), k^{*2}, of the medium defined by the relation $k^{*2}\langle\varphi(\mathbf{x})\rangle = K$.

Our aim here is to derive certain bounds on k^{*2}, using variational formulations of the problem (1). The bounds thus derived will be counterparts of the well-known Beran's bounds for the effective scalar conductivity of a random medium [2]. Four statistical parameters enter the bounds and we show how to evaluate them for the Miller's cellular medium. The respective calculations for random dispersions of spheres are being dealt with and the final results will be reported elsewhere.

PRIMAL VARIATIONAL PRINCIPLE AND UPPER BOUNDS

The random equation (1) is first replaced by the primal variational principle

$$W(\mathbf{e},\varphi)=\Big\langle \mathbf{e}(\mathbf{x})\cdot\mathbf{e}(\mathbf{x})+k^2(\mathbf{x})\varphi^2(\mathbf{x})-2K\varphi(x)\Big\rangle\to\inf. \tag{2a}$$

The functional W is considered over the class of admissible pairs

$$\mathcal{A}=\Big\{(\mathbf{e},\varphi)\ \Big|\ \mathbf{e}=\nabla\varphi\Big\}. \tag{2b}$$

Moreover,

$$\inf_{\mathcal{A}} W=-\frac{K^2}{k^{*2}}, \tag{2c}$$

and this value is attained on the pair $(\nabla\varphi,\varphi)\in\mathcal{A}$, where the field $\varphi(\mathbf{x})$ solves equation (1). The principle (2) obviously allows to obtain upper bounds on k^{*2} provided appropriate classes of trial fields are introduced.

After [3] we choose here the class of trial fields of the form

$$\varphi(\mathbf{x})=\Phi_0+\int\Phi_1(\mathbf{x}-\mathbf{y})\delta k^2(\mathbf{y})\,d^3\mathbf{y}, \tag{3}$$

where $\Phi_0=\text{const}$ and $\Phi_1(\mathbf{x})$ are nonrandom adjustable quantities, $\delta k^2(\mathbf{y})=k^2(\mathbf{y})-\langle k^2\rangle$ is the fluctuating part of the field $k^2(\mathbf{y})$. (Hereafter, the integrals are taken over the whole $\mathbb{R}^3$, if the integration domain is not explicitly indicated.) The scalar Φ_0 and the function $\Phi_1(\mathbf{x})$ are interrelated:

$$\Phi_0=\frac{1}{\langle k^2\rangle}\Big\{K-\int\Phi_1(\mathbf{y})M_2^k(\mathbf{y})\,d^3\mathbf{y}\Big\},\quad M_2^k(\mathbf{y})=\langle\delta k^2(\mathbf{0})\delta k^2(\mathbf{y})\rangle, \tag{4}$$

since the fields (3) should satisfy the equation $\langle k^2(\mathbf{x})\varphi(\mathbf{x})\rangle=K$ which follows from (1) after averaging.

Note that if $\Phi_1(\mathbf{y})=0$, then the variational principle (2) brings forth the obvious Voigt-type estimate

$$k^*\le k_V,\quad k_V=\sqrt{\langle k^2\rangle}. \tag{5}$$

On introducing (3) into (2) and taking (4) into account, we make W an usual functional of the kernel $\Phi_1(\mathbf{x})$. The minimization of the latter with respect to Φ_1 yields a certain complicated integro-differential equation which will be discussed elsewhere. Instead we shall resort here to the Ritz type procedure in which the kernel $\Phi_1(\mathbf{x})$ is taken proportional to $\dfrac{1}{4\pi|\mathbf{x}|}\exp(-k_V|\mathbf{x}|)$. Thus we minimize the functional (2) over the class of trial fields

$$\varphi(\mathbf{x})=\Phi_0+\lambda\int\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\exp(-k_V|\mathbf{x}-\mathbf{y}|)\delta k^2(\mathbf{y})\,d^3\mathbf{y}, \tag{6}$$

where now Φ_0 and λ are adjustable scalars, subject to the constraint

$$\Phi_0+\lambda\frac{M_2^k(\mathbf{0})}{\langle k^2\rangle^2}I_2^k=\frac{K}{\langle k^2\rangle}, \tag{7}$$

cf. (4), and I_2^k is a dimensionless statistical parameter for the medium, defined as follows

$$I_2^k=\frac{\langle k^2\rangle}{M_2^k(\mathbf{0})}\int\frac{1}{4\pi|\mathbf{y}|}\exp(-k_V|\mathbf{y}|)M_2^k(\mathbf{y})\,d^3\mathbf{y}. \tag{8a}$$

The procedure is now straightforward. We insert (6) into the functional W, cf. (2), and take into account (7). This makes W a quadratic function of λ whose minimization yields an upper bound on k^{*2}, namely

$$\frac{k^{*2}}{k_V^2} \le 1 - \frac{\dfrac{M_2^k(\mathbf{0})}{\langle k^2\rangle^2}(I_2^k)^2}{I_2^k + \dfrac{M_3^k(\mathbf{0},\mathbf{0})}{\langle k^2\rangle M_2^k(\mathbf{0})} I_3^k}, \tag{9}$$

where I_3^k is another dimensionless statistical parameter for the medium:

$$I_3^k = \frac{\langle k^2\rangle^2}{M_3^k(\mathbf{0},\mathbf{0})} \iint \frac{1}{16\pi^2|\mathbf{y}_1||\mathbf{y}_2|} \exp(-k_V(|\mathbf{y}_1| + |\mathbf{y}_2|)) M_3^k(\mathbf{y}_1,\mathbf{y}_2)\, d^3\mathbf{y}_1\, d^3\mathbf{y}_2; \tag{8b}$$

here $M_3^k(\mathbf{y}_1,\mathbf{y}_2) = \langle \delta k^2(\mathbf{0})\delta k^2(\mathbf{y}_1)\delta k^2(\mathbf{y}_2)\rangle$ is the three-point correlation function.

Note that the integrand's kernel in the r.h.-side of equation (6) is proportional to that that appears in the first-order term in the perturbation solution of the problem (1) in the case of a weakly inhomogeneous medium. A variational procedure, based on the similar term of the perturbation solution in the scalar conductivity problem, was developed by Beran [2]. That is why the bound (9), as well as the respective lower bound below, could be viewed as counterparts of Beran's bounds for the absorption problem under study.

DUAL PRINCIPLE AND LOWER BOUNDS

The construction of the dual variational principle for the problem under consideration needs evaluation of the Fenchel-Young transform of the functional W, cf., e.g., [4]. Skipping all details, we give only the eventual formulation[1]

$$J(\mathbf{e},\varphi) = -\Big\langle \mathbf{e}^*(\mathbf{x})\cdot\mathbf{e}^*(\mathbf{x}) + \alpha^2(\mathbf{x})(\varphi^*(\mathbf{x}) + K)^2 \Big\rangle \to \sup\,. \tag{10a}$$

where $\alpha^2(\mathbf{x}) = 1/k^2(\mathbf{x})$ is the "compliance" field. The functional J is considered over the class of admissible pairs

$$\mathcal{A}^* = \Big\{ (\mathbf{e}^*,\varphi^*) \;\Big|\; \langle \mathbf{e}^*\rangle = 0,\ \nabla\cdot\mathbf{e}^* = \varphi^* \Big\}. \tag{10b}$$

Moreover,

$$\inf_{\mathcal{A}} W = \sup_{\mathcal{A}^*} J = -\frac{K^2}{k^{*2}}, \tag{10c}$$

and the supremum value of the functional J is attained on the pair $(\mathbf{e}^*,\varphi^*) \in \mathcal{A}^*$, for which $\mathbf{e}^* = \nabla\varphi$, $\varphi^*(\mathbf{x}) = k^2(\mathbf{x})(\varphi(\mathbf{x}) + K)$, where the field $\varphi(\mathbf{x})$ solves equation (1). The principle (10) obviously allows to obtain upper bounds on k^{*2} provided appropriate classes of trial fields are introduced. For instance, in the simplest case when both $\mathbf{e}^*$ and φ^* vanish, one gets the Reuss-type estimate

$$k_R \le k^*, \quad 1/k_R = \sqrt{\langle \alpha^2\rangle}. \tag{11}$$

The counterpart of the class (6) now is

$$\mathbf{e}^*(\mathbf{x}) = \lambda\nabla_x \int \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \exp(-k_R|\mathbf{x}-\mathbf{y}|)\delta\alpha^2(\mathbf{y})\, d^3\mathbf{y}, \tag{12}$$

[1]One of the authors (KM) gratefully acknowledges the helpful discussion with J. Willis, concerning the formulation of the dual principle for the problem under study.

where $\lambda \in \mathbb{R}$ is adjustable scalar and $\delta\alpha^2(\mathbf{x}) = \alpha^2(\mathbf{x}) - \langle\alpha^2(\mathbf{x})\rangle$ is the fluctuation of the "compliance" field. Note that the kernels in the classes (6) and (12) differ, because the Voigt and Reuss values, k_V and k_R, are used within the respective exponential functions.

On inserting (12) into the functional (10a) and using the fact that $\nabla \cdot \mathbf{e}^* = \varphi^*$, we make J a quadratic function of λ whose minimization yields a lower bound on k^{*2}, namely

$$\left\{ 1 - \frac{\dfrac{M_2^\alpha(\mathbf{0})}{\langle\alpha^2\rangle^2}(I_2^\alpha)^2}{I_2^\alpha + \dfrac{M_3^\alpha(\mathbf{0},\mathbf{0})}{\langle\alpha^2\rangle M_2^\alpha(\mathbf{0})} I_3^\alpha} \right\}^{-1} \leq \frac{k^{*2}}{k_R^2}, \tag{13}$$

where

$$I_2^\alpha = -\frac{1}{M_2^\alpha(\mathbf{0})} \int \Delta_y \left(\frac{1}{4\pi|\mathbf{y}|} \exp(-k_R|\mathbf{y}|) \right) M_2^\alpha(\mathbf{y})\, d^3\mathbf{y}, \tag{14a}$$

$$I_3^\alpha = \frac{1}{M_3^\alpha(\mathbf{0},\mathbf{0})} \iint \Delta_{y_1} \left(\frac{1}{4\pi|\mathbf{y}_1|} \exp(-k_R|\mathbf{y}_1|) \right)$$

$$\times\, \Delta_{y_2} \left(\frac{1}{4\pi|\mathbf{y}_2|} \exp(-k_R(|\mathbf{y}_2|) \right) M_3^\alpha(\mathbf{y}_1,\mathbf{y}_2)\, d^3\mathbf{y}_1\, d^3\mathbf{y}_2, \tag{14b}$$

are the counterparts of dimensionless statistical parameters (8) that enter the upper bound for the medium, and

$$M_2^\alpha(\mathbf{y}) = \langle \delta\alpha^2(\mathbf{0})\delta\alpha^2(\mathbf{y})\rangle, \quad M_3^\alpha(\mathbf{y}_1,\mathbf{y}_2) = \langle \delta\alpha^2(\mathbf{0})\delta\alpha^2(\mathbf{y}_1)\delta\alpha^2(\mathbf{y}_2)\rangle$$

are, respectively, the two- and three-point correlation functions for the field $\alpha(\mathbf{y})$.

BOUNDS FOR CELLULAR MEDIA

Let us recall that a simple and plausible random geometry for a two-phase medium has been proposed by Miller [5]. This is the so-called cellular material which is obtained by dividing the space into closed regions, called cells. Afterwards the cells are randomly filled up with one of the two constituents possessing (in our context) absorption coefficients k_f^2 or k_m^2. The volume fractions of the latter are respectively c_f or c_m, see [5], [6] for more details.

Under the assumption of statistical isotropy, the two-and three-point for such a cellular medium have the form [6]:

$$M_2^k(\mathbf{y}) = c_f c_m [k^2]^2 \frac{1}{V_a} \int h(\mathbf{y}) h(\mathbf{y}-\mathbf{z})\, d^3\mathbf{z},$$

$$M_3^k(\mathbf{y}_1,\mathbf{y}_2) = c_f c_m (c_m - c_f)[k^2]^3 \frac{1}{V_a} \int h(\mathbf{z}) h(\mathbf{y}_1-\mathbf{z}) h(\mathbf{y}_2-\mathbf{z})\, d^3\mathbf{z}, \tag{15}$$

where $h(\mathbf{x})$ denotes the characteristic function of the mean cell, assumed spherical with radius a, $V_a = \frac{4}{3}\pi a^3$ is its volume and $[k^2] = k_f^2 - k_m^2$. Similar expressions hold for the "compliance" field $\alpha^2(\mathbf{x}) = 1/k^2(\mathbf{x})$, with the only replacement of $[k^2]$ by $[\alpha^2] = \alpha_f - \alpha_m$, $\alpha_f = 1/k_f$, $\alpha_m = 1/k_m$.

On introducing (15) into the definitions (8a) and (8b) of the statistical parameters I_2^k and I_3^k respectively, one gets integrals involving the Helmholtz potential $\chi_V = h * \dfrac{1}{4\pi|\mathbf{x}|} \exp(-k_V|\mathbf{x}|)$

for a single sphere of radius a, located at the origin. Using the simple analytical form of the latter, the following expressions for these parameters are eventually obtained:

$$I_2^k = 1 - F_2(a_V), \quad I_3^k = 1 - 2F_2(a_V) + F_3(a_V), \tag{16a}$$

where a_V is the dimensionless parameter $a_V = ak_V$ and

$$F_2(x) = 3\frac{1+x}{x^3}\exp(-x)(x\cosh x - \sinh x),$$

$$F_3(x) = \frac{3}{2}\frac{(1+x)^2}{x^3}\exp(-2x)(\sinh x\cosh x - x). \tag{17}$$

Similar calculations for the statistical parameters I_2^α and I_3^α, that enter the lower bound (13), involve the Helmholtz potential $\chi_R = h * \dfrac{1}{4\pi|\mathbf{x}|}\exp(-k_R|\mathbf{x}|)$ for a sphere of radius a, located at the origin. It appears finally that

$$I_2^\alpha = F_2(a_R), \quad I_3^\alpha = F_3(a_R), \tag{16b}$$

where $a_R = ak_R$ and the functions F_2 and F_3 are given in (17).

Thus the Beran's type bounds on the effective absorption coefficient of a cell medium could be summarized as follows

$$k_R^2\left\{1 - \frac{c_f c_m(\delta\alpha)^2(I_2^\alpha)^2}{I_2^\alpha + \delta\alpha(c_m - c_f)I_3^\alpha}\right\}^{-1} \le k^{*2} \le k_V^2\left\{1 - \frac{c_f c_m(\delta k)^2(I_2^k)^2}{I_2^k + \delta k(c_m - c_f)I_3^k}\right\}, \tag{18}$$

where $\delta k = \dfrac{[k^2]}{\langle k^2\rangle}$ and $\delta\alpha = \dfrac{[\alpha^2]}{\langle\alpha^2\rangle}$; the needed statistical parameters are defined in equations (16a,b).

Note that $F_2(x)$ and $F_3(x)$ are monotonically increasing functions of x and $F_2(0) = F_3(0) = 0$, $F_2(\infty) = F_3(\infty) = 1$. That is why the four statistical parameters I_2^k, I_3^k, I_2^α and I_3^α for a cellular medium always lie in the interval $[0, 1]$.

Tables 1 and 2 illustrate the performance of the bounds (18) for a cellular medium at $a_m = 1$ and $a_m = 10$, respectively, where $a_m = ak_m$. It is well seen that the bounds remain tolerably close and supply useful information about k^{*2} even when the absorption ability of one of the constituents is one hundred times greater than that of the other ($k_f^2/k_m^2 = 100$ or 0.01). Naturally enough, one of the bounds degenerates in the limiting cases $k_f^2/k_m^2 \to 0$ or $k_f^2/k_m^2 \to \infty$.

TABLE 1

Values of the bounds (18) on k^{*2}/k_m^2 for a cellular medium at $a_m = 1$.

	$k_f^2/k_m^2 = 0.01$		$k_f^2/k_m^2 = 100$	
c_f	lower	upper	lower	upper
0	1	1	1	1
0.05	0.936	0.940	1.268	1.559
0.10	0.873	0.881	1.570	2.251
0.25	0.694	0.710	2.734	4.842
0.50	0.431	0.449	6.318	12.019
0.75	0.205	0.214	16.379	28.674
0.90	0.085	0.087	34.390	54.724
0.95	0.047	0.048	46.055	71.883
1	0.01	0.01	100	100

TABLE 2

Values of the bounds (18) on k^{*2}/k_m^2 for a cellular medium at $a_m = 10$.

	$k_f^2/k_m^2 = 0.01$		$k_f^2/k_m^2 = 100$	
c_f	lower	upper	lower	upper
0	1	1	1	1
0.05	0.461	0.719	1.063	1.138
0.10	0.344	0.547	1.134	1.258
0.25	0.164	0.287	1.402	1.694
0.50	0.063	0.120	2.205	3.004
0.75	0.027	0.048	4.502	6.839
0.90	0.016	0.023	10.484	16.819
0.95	0.013	0.016	18.623	29.443
1	0.01	0.01	100	100

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