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ON THE CLUSTER BOUNDS FOR THE EFFECTIVE PROPERTIES OF MICROCRACKED SOLIDS

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ABSTRACT

The paper is concerned with the problem of predicting macroscopic properties of solids, containing randomly distributed penny-shaped microcracks. It is proposed to employ the formalism of marked sets of random points, treating the mark as orientation of the crack located at a given point. As a first and simplest application of this approach the so-called first-order cluster bound of Torquato (1986 *J. Chem. Phys.* **84,** 6345–6359) on the effective scalar conductivity is derived. It turns out that the bound does not depend on the two- and three-point statistics of the distribution of cracks, unlike the case of dispersions of spheres or spheroids. The "optimality" of the bound within a much wider class of "cluster type" trial fields is demonstrated. In the elastic case the cluster bounds are explicitly derived as well, and are again found to be independent of cracks' statistics. In both scalar and elastic cases the bounds coincide with the so-called "approximation of non-interacting cracks" thus rigorously proving that for the assumed isotropic cracks' statistics the interactions always decrease the conductivity and the elastic moduli of a microcracked solid.

1. INTRODUCTION

The paper is devoted to the problem of the macroscopic behaviour of solids, containing randomly distributed penny-shaped microcracks. As is well known, the literature on this subject is extensive, and many of the basic references can be found in the comprehensive review paper of Kachanov (1992) [see also Section II.6 of the book of Nemat-Nasser and Hori (1993) for an elucidating introduction]. We shall point out only that there exist two main approaches to the problem that differ, above all, in the way the cracks are introduced and treated. The first one, adopted, e.g., in the pioneering works of Bristow (1960), Walsh (1965), Budiansky and O'Connell (1976) and many others, deals directly with the singular stress field generated by a single crack, considered as a cut [or a slit in 2-D] along a surface within the

body. For example, in the dilute case the change of the elastic energy introduced by a single crack has been used to produce rigorous results, in the first order in crack density, for the overall elastic moduli of a solid (Bristow, 1960; Walsh, 1965). However, this approach invokes from the very beginning a number of specific notions and results from fracture mechanics such as energy release rate, stress concentration factors, etc. The second approach addresses first the more general situation concerning the overall behaviour of a random [or aligned] dispersion of oblate spheroids and then, in the obtained results, the "crack" limit is taken in which the aspect ratio of the spheroids tends to zero and hence they degenerate into penny-shaped cracks in 3-D [or just slits in 2-D]. This approach has been advocated and successfully utilized by a number of authors, to mention only Willis (1977), Benveniste (1987), Huang *et al.* (1993) and recently by Ponte Castañeda and Willis (1995). In the author's view this second approach is preferable and more fruitful in general [apart from the possibility to treat in an entirely similar manner short-fiber composites by modelling them again as dispersions of spheroids, but prolate]. The reason is that the theory of microcracked solids can be naturally included in this way within the more general and widely examined theory of two-phase particulate media as a simple [at least conceptually if not technically] limiting particular case. In turn all the general and intuitively appealing ideas from mechanics of such media which try to incorporate, to some extent, inclusion interactions—self-consistency (Budiansky and O'Connell, 1976), differential scheme (Hashin, 1988), Mori-Tanaka method (Benveniste, 1985, 1987), etc.—can be easily recast and adapted for a microcracked solid in the "crack" limit. With similar ease the variational bounds on the effective properties of dispersions of spheroids, derived by Willis (1977, 1980) and Ponte Castañeda and Willis (1995), using the Hashin-Shtrikman (HS) variational principle (Hashin and Shtrikman, 1962), produce in the "crack" limit rigorous and nontrivial estimates on the effective properties of microcracked solids.

The second approach has one more advantage that we want to emphasize and exploit to a certain extent here. Namely, it allows us to introduce the useful formalism of marked sets of random points into the theory of microcracked solids. The basic idea is simple and physically clear: each spheroid is specified by a random point—its center—to which a "mark" that describes its orientation is associated. Then, from a statistical point of view, the dispersion is characterized by the random density field of a type of Stratonovich (1963). This allows in turn use of the formalism of functional [Volterra-Wiener] series as employed by the author in a number of studies (Markov, 1991; Markov and Zvyatkov, 1991, 1995; Markov and Christov, 1992, *et al.*). Details and the needed formulae are given in Section 2. As a nontrivial application of this formalism the evaluation of the so-called cluster bound of Torquato (1986) and a certain generalization will be addressed here. This bound follows from the classical variational principle if one uses trial fields formed as superpositions of the single inclusion [i.e. single spheroid] fields, multiplied by an adjustable scalar parameter. To this end it is necessary that the single spheroid field be recalled in Section 3 in the scalar context, focusing on its asymptotic form in the above mentioned "crack" limit. The variational procedure in the "marked" case is discussed in Section 4, where first the cluster bound is derived in a general form containing the two- and three-point probability densities for the random set of cracks' centers. The explicit form of the bound is evaluated in the scalar context in Section 5 which, from a formal and technical point of view is central for the paper. In Section 6 a

natural generalization of the cluster bound is discussed in which the single spheroid solution is replaced by an adjustable kernel. The central result there is the fact that this bound cannot be improved, if much wider class of trial fields is employed. The most curious finding, however, is that the cluster bound does not feel both two- and three-point crack statistics, depending only on crack density. Treating the elastic case is conceptually and technically straightforward and is very briefly discussed in Sections 7 and 8. The cluster bounds on the effective bulk and shear moduli in this case coincide [in 3-D] with the prescriptions of the so-called "approximation of non-interacting cracks" or, which is the same, with the prescriptions of the Mori-Tanaka type approximation [see Benveniste, 1987 and especially, the review papers of Kachanov, 1992], being again independent of the statistics. This rigorously proves that for the assumed isotropic cracks' statistics the interactions always decrease the conductivity and the elastic moduli of a microcracked solid. The concluding Section 9 contains a brief discussion of plausible reasons for the observed independence of statistics of the cluster bounds, as well as some of the possible further generalizations of the approach.

2. RANDOM DISPERSIONS OF SPHEROIDS

Consider a random array of identical and nonoverlapping oblate spheroids with semiaxes $a = b > c$. The array is assumed statistically homogeneous. The spatial orientation $\boldsymbol{\omega}$ of each spheroid is specified by the unit vector $\mathbf{e}_3 = \mathbf{e}_\omega$ directed along the shortest semiaxis c. The array is uniquely determined by the set $\mathcal{S} = \left\{\mathbf{x}_j, \boldsymbol{\omega}_j\right\}$, comprising the location $\mathbf{x}_j \in \mathbb{R}^3$ of the jth spheroid center and its orientation $\boldsymbol{\omega}_j \in \Omega$; hereafter $\Omega = \{\mathbf{z} \in \mathbb{R}^3 \mid |\mathbf{z}| = 1\}$ denotes the unit sphere in $\mathbb{R}^3$. The arguments in the sequel will be fully similar in the 2-D case, when the spheroids are replaced by aligned elliptical cylinders whose cross-sections have semiaxes a and c, $a > c$. The orientations $\boldsymbol{\omega}$ of the ellipses are specified again by the unit normal vectors $\mathbf{e}_2 = \mathbf{e}_\omega$, directed along the shorter semiaxis, which span this time the unit circle $\Omega = \{\mathbf{z} \in \mathbb{R}^2 \mid |\mathbf{z}| = 1\}$ in $\mathbb{R}^2$, centered at the origin. For brevity, we shall sometimes speak of spheroids in the 2-D case as well.

The set $\mathcal{S}$ can be treated as a marked system of random points in the sense that with each point $\mathbf{x}_j$ its "mark" $\boldsymbol{\omega}_j$ is associated, interpreted here as the orientation of the spheroid, located at $\mathbf{x}_j$. [For the general definition and basic properties of sets of marked random points see Snyder (1975).]

The set $\mathcal{S}$ is defined statistically by the multipoint probability densities F_k such that

$$dP = F_k(\mathbf{y}_1, \ldots, \mathbf{y}_k; \boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_k)\, \mathrm{d}\mathbf{y}_1 \ldots \mathrm{d}\mathbf{y}_k\, \mathrm{d}S_{\Omega_1} \ldots \mathrm{d}S_{\Omega_k} \tag{2.1}$$

is the probability to find simultaneously in the vicinities $\mathbf{y}_i < \mathbf{y} < \mathbf{y}_i + \mathrm{d}\mathbf{y}_i$ of the spatial positions $\mathbf{y}_i$, k members of the system with marks (i.e. with orientations) $\boldsymbol{\omega} \in \Omega$, whose end points lie in the vicinities $\mathrm{d}S_{\Omega_i}$ of the points $\boldsymbol{\omega}_i \in \Omega$, respectively ($i = 1, \ldots, k$). The condition of nonoverlapping yields certain restrictions on the functions F_k which would be quite complicated in general, especially if there exists a spatial correlation between location and orientation of the spheroids.

We shall adopt, however, the first of our basic simplifying assumptions, namely, that there is no such correlation, i.e. spatial location and orientation are statistically independent. Then

the probability density functions factorize

$$F_k(\mathbf{y}_1, \ldots, \mathbf{y}_k; \boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_k) = f_k(\mathbf{y}_1, \ldots, \mathbf{y}_k)\, P_k(\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_k). \tag{2.2}$$

The no long-range order hypothesis is assumed (Willis, 1981), so that $f_k(\mathbf{y}_1, \ldots, \mathbf{y}_k) \to n^k$ when $|\mathbf{y}_i - \mathbf{y}_j| \to \infty$, for all $i, j = 1, 2, \ldots k$, $i \neq j$, $k \geq 2$, and n is the number density of the spheroids.

The second basic assumption, adopted hereafter, is that the spatial orientation of different spheroids is also statistically independent—the orientation of a given spheroid does not influence the orientation of any of the rest. This means that the mark density functions P_k factorize as well

$$P_k(\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_k) = P(\boldsymbol{\omega}_1) \ldots P(\boldsymbol{\omega}_k), \tag{2.3}$$

for any k.

A simple condition that suffices (but is not necessary of course) to forbid overlapping of cracks reads, in terms of the functions f_k, as

$$f_k(\mathbf{y}_1, \ldots, \mathbf{y}_k) = 0, \quad \text{if} \quad |\mathbf{y}_i - \mathbf{y}_j| \leq 2a \quad \text{for a pair} \quad i \neq j, \tag{2.4}$$

$(i, j = 1, \ldots, k)$, since, if the centers of two spheroids lie closer than $2a$, their orientations cannot be mutually independent due to the fact that overlapping is forbidden. The condition (2.4) is assumed by many authors, e.g., by Kanaun (1980) or Ponte Castañeda and Willis (1995). As pointed out by Kachanov (1992, p. 324), its imposition makes the effective moduli of the microcracked solid a bit "softer," since crack configurations of shielded type, say, closely located parallel cracks, are excluded. This fact is also corroborated by Kanaun's approximate scheme (Kanaun, 1980) in which the values of the effective properties for a solid, containing a Poissonian system of cracks, do decrease, if the nonoverlapping assumption is additionally imposed.

Note that the assumption (2.4) can be simply interpreted in the following manner. Insert each spheroid within a sphere of radius a, both having a common center. Equation (2.4) then means that the so appearing spheres are impenetrable and hence their volume fraction is $\alpha_d = nV_a$, i.e.

$$\alpha_3 = \tfrac{4}{3}\pi n a^3 \quad \text{(in 3-D)} \quad \text{or} \quad \alpha_2 = \pi n \alpha^2 \quad \text{(in 2-D)}; \tag{2.5}$$

recall that n is the number density of the spheroids. Since the maximum packing value for impenetrable spheres is close to 0.65 – 0.7 in both 3-D or 2-D cases, the theory that follows is realistic, concerning realizable random distributions, only at values of α_d not exceeding these maximum packing values. Hence, to be on the safe side, we shall assume in the sequel that $\alpha_d \leq 0.6$. Though the basic ideas of the approach herein proposed are applicable for higher values of α_d as well, the price is severe: Allowing the above mentioned spheres to intersect, one has to reject immediately the factorization assumptions (2.2) and (2.3) and to take into account the fact that if, say, the centers of two spheroids are closer than $2a$, not all of their orientations are realizable, due to the nonoverlapping assumption. The resulting analysis, if analytically tangible at all, would be extremely cumbersome.

Another interpretation of (2.4) is that the spheroid, centered at $\mathbf{x}_j$ is surrounded by a "security" sphere of the radius $2a$, also centered at $\mathbf{x}_j$, such that the centers of the rest of

the spheroids are forbidden to fall within this sphere, for all $j = 1, 2, \ldots$. Note that a more general situation, when the spheroids can be prolate as well and their spatial distribution possesses macroscopic symmetry of a similar ellipsoidal type, has been recently treated by Ponte Castañeda and Willis (1995), using earlier ideas of Willis (1977).

The statistical homogeneity of the array under study yields, in particular,

$$F_1(\mathbf{y}, \boldsymbol{\omega}) = nP(\boldsymbol{\omega}). \tag{2.6}$$

The function $P(\boldsymbol{\omega})$ satisfies the obvious condition

$$\int_\Omega P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} = 1.$$

Moreover, we shall assume that there is no preferable orientation of the spheroids, which means that

$$P(\boldsymbol{\omega}) = \frac{1}{4\pi} \quad \text{(in 3-D)} \quad \text{or} \quad P(\boldsymbol{\omega}) = \frac{1}{2\pi} \quad \text{(in 2-D)}. \tag{2.7}$$

A convenient statistical description of the set $\mathcal{S}$, corresponding to the array of spheroids under study, is the marked random density function of the type of Stratonovich (1963)

$$\psi(\mathbf{x}; \boldsymbol{\omega}) = \sum_j \delta(\mathbf{x} - \mathbf{x}_j)\, \delta(\boldsymbol{\omega} - \boldsymbol{\omega}_j). \tag{2.8}$$

The moments of the field $\psi(\mathbf{x}; \boldsymbol{\omega})$ can be expressed by the multipoint probability densities F_k and vice versa; the general formulae are given in Stratonovich (1963) [in the "non-marked" case, but their generalization to the "marked" one is straightforward and causes no problems]. Under the simplifying assumptions (2.2) and (2.3) the first few moments of $\psi(\mathbf{x}; \boldsymbol{\omega})$, needed in what follows, are

$$\begin{aligned}
\langle \psi(\mathbf{y}; \boldsymbol{\omega}) \rangle &= F_1(\mathbf{y}; \boldsymbol{\omega}) = nP(\boldsymbol{\omega}), \\
\langle \psi(\mathbf{y}_1; \boldsymbol{\omega}_1) \psi(\mathbf{y}_2; \boldsymbol{\omega}_2) \rangle &= nP(\boldsymbol{\omega}_1)\delta(\mathbf{y}_{1,2})\delta(\boldsymbol{\omega}_{1,2}) + f_2(\mathbf{y}_{1,2})P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2), \\
\langle \psi(\mathbf{y}_1; \boldsymbol{\omega}_1) \psi(\mathbf{y}_2; \boldsymbol{\omega}_2) \psi(\mathbf{y}_3; \boldsymbol{\omega}_3) \rangle &= nP(\boldsymbol{\omega}_1)\delta(\mathbf{y}_{1,2})\delta(\mathbf{y}_{1,3})\delta(\boldsymbol{\omega}_{1,2})\delta(\boldsymbol{\omega}_{1,3}) \\
+3 \left\{ f_2(\mathbf{y}_{1,2})P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)\delta(\mathbf{y}_{1,3})\delta(\boldsymbol{\omega}_{1,3}) \right\}_s &+ f_3(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)P(\boldsymbol{\omega}_3),
\end{aligned} \tag{2.9}$$

etc., where $\left\{ \cdot \right\}_s$ denotes symmetrization [more precisely, one third of the sum of the three terms obtained by means of the cyclic change $1 \to 2 \to 3 \to 1$ of the indices in the brackets]. For brevity hereafter we denote $\mathbf{y}_{i,j} = \mathbf{y}_i - \mathbf{y}_j$ and $\boldsymbol{\omega}_{i,j} = \boldsymbol{\omega}_i - \boldsymbol{\omega}_j$; due to the assumed statistical homogeneity $f_2(\mathbf{y}_1, \mathbf{y}_2) = f_2(\mathbf{y}_1 - \mathbf{y}_2)$.

The microcracked solids in 3-D in the sequel, as already pointed out, will be viewed as limiting cases of solids, containing spheroidal cavities when the aspect ratio $w = c/a \to 0$. Similarly, in 2-D we shall deal with a solid containing aligned elliptical cavities and take again the limit as $w = c/a \to 0$, assuming the external traction to be applied perpendicularly to the cylinders' axes. In the quest for the effective behaviour of such solids, we shall encounter certain quantities depending on the aspect ratio w, averaged over all possible orientations of the spheroids. The basic interest for us will lie in the limits of these quantities when $w \to 0$, i.e. when the cavities degenerate into cracks [penny-shaped in 3-D and aligned cylindrical

ones in 2-D]. The needed limits can be easily found, as it will be seen, making use of the following basic lemma.

Lemma 2.1. Let $h_\omega(\mathbf{x}) = h(\mathbf{x};\boldsymbol{\omega})$ be the characteristic function of a spheroid located at the origin, with the orientation $\boldsymbol{\omega}$. Then in $\mathbb{R}^d$ $(d = 2, 3)$, and under the assumption (2.7),

$$\lim_{w\to 0} \frac{1}{w} \int_\Omega h(\mathbf{x};\boldsymbol{\omega})\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} = H_d(\rho)\, h_a(\mathbf{x}), \tag{2.10a}$$

where $h_a(\mathbf{x})$ is the characteristic function of a sphere [in 3-D] or of a disk [in 2-D] of radius a, located at the origin, $\rho = r/a$, $r = |\mathbf{x}|$, and

$$H_d(\rho) = \frac{b_d}{\rho}\sqrt{1-\rho^2}, \quad b_d = \begin{cases} \dfrac{2}{\pi} & \text{in 2-D,} \\ 1 & \text{in 3-D.} \end{cases} \tag{2.10b}$$

Note that the explicit form of the function $H_d(\rho)$ is given here for the sake of completeness only since it will not be needed in the present study. Only the following property

$$\int_{S_a} H_2(\rho)\, \mathrm{d}\mathbf{x} = S_a \ \ \text{(in 2-D)} \quad \text{or} \quad \int_{V_a} H_3(\rho)\, \mathrm{d}\mathbf{x} = V_a \ \ \text{(in 3-D)} \tag{2.11}$$

of $H_d(\rho)$ will be repeatedly used. [It can be deduced immediately from equation (2.10a), if one integrates both sides of the latter over the unit disk [or ball], noticing that $\int h(\mathbf{x};\boldsymbol{\omega})\, \mathrm{d}\mathbf{x}$ equals the volume of the appropriate ellipse (or ellipsoid)]. A simple geometrical proof of Lemma 2.1 will be given elsewhere.

Corollary 2.1. Let $\mathbf{e}_\omega$ be the unit vector along the shorter semiaxis c of the ellipsoid or ellipse in the 3-D and 2-D cases respectively. Then in $\mathbb{R}^d$ $(d = 2, 3)$

$$\lim_{w\to 0} \frac{1}{w} \int_\Omega \mathbf{e}_\omega \mathbf{e}_\omega\, h(\mathbf{x};\boldsymbol{\omega})\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} = \frac{1}{d-1}\, h_a(\mathbf{x})\, H_d(\rho)\, r\, \nabla\nabla\, r, \tag{2.12}$$

with the notations used in Lemma 2.1.

Proof. Due to obvious symmetry, the second-rank tensor in the left-hand side of (2.12) has the form $h_a(\mathbf{x})\, A(r)\, [\, \mathbf{I} - B(r)\, \mathbf{e}_r \mathbf{e}_r\,]$, with $\mathbf{I}$ denoting the unit second-rank tensor, $\mathbf{e}_r = \mathbf{x}/r$. It is clear on the other hand that, in the limit $w \to 0$, $h(\mathbf{x}, \boldsymbol{\omega}) \neq 0$ only for $\mathbf{e}_r \perp \mathbf{e}_\omega$ which implies that $B(r) = 1$. A simple contraction then immediately yields (2.12), taking into account (2.11) and the formulae $\mathbf{I} - \mathbf{e}_r\, \mathbf{e}_r = r\, \nabla\nabla\, r$, $\mathrm{tr}\, (\, \mathbf{I} - \mathbf{e}_r\, \mathbf{e}_r\,) = r\, \Delta r = d - 1$.

3. THE SINGLE SPHEROID FIELD AND ITS AVERAGING

Denote by $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ the disturbance to the temperature field $\mathbf{G}\cdot\mathbf{x}$ in an unbounded matrix of conductivity κ_m, produced by the presence of a single spheroidal inhomogeneity S_ω of conductivity κ_f, located at the origin. The field $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ is the continuous and everywhere bounded solution of the equation

$$\kappa_m \Delta T^{(1)}(\mathbf{x};\boldsymbol{\omega}) + [\kappa]\nabla\cdot\Big\{h(\mathbf{x};\boldsymbol{\omega})[\mathbf{G} + \nabla T^{(1)}(\mathbf{x};\boldsymbol{\omega})]\Big\} = 0, \quad [\kappa] = \kappa_f - \kappa_m. \tag{3.1}$$

As is well-known, the gradient $\nabla T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ is constant within S_ω

$$\nabla T^{(1)}(\mathbf{x};\boldsymbol{\omega}) = \mathbf{B}(\boldsymbol{\omega})\cdot\mathbf{G}, \quad \mathbf{x}\in S_\omega. \tag{3.2}$$

The second rank tensor $\mathbf{B}(\boldsymbol{\omega})$ [we underline its dependence on the orientation $\boldsymbol{\omega}$] is well-known [see, e. g., the book of Mura, 1988], and it has the form

$$\mathbf{B}(\boldsymbol{\omega}) = \mathbf{A}(\boldsymbol{\omega}) - \mathbf{I}, \quad \mathbf{A}(\boldsymbol{\omega}) = \left(\mathbf{I} + [\kappa]\,\mathbf{P}\right)^{-1}, \quad \mathbf{P} = -\frac{1}{\kappa_m}\,\nabla\nabla\,\varphi_\omega, \tag{3.3}$$

where $\mathbf{P}$ is the so-called $\mathbf{P}$-tensor for the case under study, when there is only one kind of inclusions, immersed into a matrix of conductivity κ_m [see, e.g., Willis, 1978], and $\varphi_\omega(\mathbf{x}) = (h_\omega * G_0)(\mathbf{x}) = \int h(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})G_0(\mathbf{y})\,\mathrm{d}\mathbf{y}$ denoting the Newtonian potential for the spheroid S_ω; $G_0(\mathbf{y})$ is the Green function for the Laplace operator in $\mathbb{R}^d$, i.e. $1/4\pi|\mathbf{x}|$ in 3-D or $-\ln|\mathbf{x}|/2\pi$ in 2-D. Recall that the potential φ_ω solves the equation $\Delta\varphi_\omega(\mathbf{x}) + h(\mathbf{x};\boldsymbol{\omega}) = 0$. An obvious consequence of the latter equation, when comparing it with (3.1) and (3.2), is that

$$T^{(1)}(\mathbf{x};\boldsymbol{\omega}) = \frac{[\kappa]}{\kappa_m}\,\mathbf{G}\cdot(\mathbf{I}+\mathbf{B}(\boldsymbol{\omega}))\cdot\nabla\varphi_\omega(\mathbf{x}). \tag{3.4}$$

In turn, citing Mura (1988) or Muratov (1975):

$$\nabla\nabla\,\varphi_\omega = -M_\perp(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2) - M\mathbf{e}_3\mathbf{e}_3, \quad \mathbf{x}\in S_\omega, \tag{3.5a}$$

where, for an oblate spheroid ($w<1$)—the only case of interest for us in this study—one has

$$M_\perp = \frac{1}{2}\,(1-M) = \frac{\pi}{4}\,w + o(w), \quad M = \frac{1}{e^2}\left(1 - \frac{w}{e}\arcsin e\right) = 1 - \frac{\pi}{2}\,w + o(w), \tag{3.5b}$$

with $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ denoting the orthonormal vectors along the semiaxes of the spheroids S_ω, such that $\boldsymbol{\omega} = \mathbf{e}_3$; $e = \sqrt{1-w^2}$ is spheroid's eccentricity. The obvious asymptotic expansions of the quantities $M_\perp$ and M in the limit $w = c/a \to 0$ are given as well in (3.5b).

Having in mind the application to microcracked solids, only the case of a spheroidal cavity will be treated hereafter, i.e. $\kappa_f = 0$. In this case

$$\mathbf{B}(\boldsymbol{\omega}) = \frac{M_\perp}{1-M_\perp}\,(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2) + \frac{M}{1-M}\,\mathbf{e}_3\mathbf{e}_3 \tag{3.6}$$

[see eqs (3.3) to (3.5)]. Hence in the limit $w = c/a \to 0$, i.e. when the cavities degenerate into penny-shaped cracks,

$$\mathbf{A}(\boldsymbol{\omega}) \sim \mathbf{B}(\boldsymbol{\omega}) = \frac{2}{\pi w}\,\mathbf{e}_3\mathbf{e}_3 + O(1) \ \text{ in 3-D}, \tag{3.7a}$$

as it easily follows from (3.5) and (3.6). The sign $\sim$ hereafter indicates that both tensors $\mathbf{A}(\boldsymbol{\omega})$ and $\mathbf{B}(\boldsymbol{\omega})$ have the same leading term in their asymptotic expansions in the limit $w \to 0$.

In 2-D, as already pointed out, instead of a spheroid, we have an elliptical cylinder with semiaxes $a > c$ of its the cross-section S_ω. Then $\nabla\nabla\,\varphi_\omega = -M_1\mathbf{e}_1\mathbf{e}_1 - M_2\mathbf{e}_2\mathbf{e}_2$, where $\mathbf{e}_1$ and $\mathbf{e}_2$ are the orthonormal vectors along the semiaxes of S_ω, such that $\mathbf{e}_2 = \mathbf{e}_\omega$ is along the shorter axis c. In the limit $w = c/a \to 0$ one has $M_1 = w + o(w)$ and $M_2 = 1 - w + o(w)$ [see again Mura, 1988, or Muratov, 1975]. In turn, according to (3.3), this means that in 2-D the tensor $\mathbf{B}(\boldsymbol{\omega})$ [at $\kappa_f = 0$ again] has in the same limit $w \to 0$ the form

$$\mathbf{A}(\boldsymbol{\omega}) \sim \mathbf{B}(\boldsymbol{\omega}) = \frac{1}{w}\,\mathbf{e}_2\mathbf{e}_2 + O(1) \quad \text{in 2-D.} \tag{3.7b}$$

The formulae (3.7a, b) can be written in both 2-D and 3-D as

$$\mathbf{A}(\boldsymbol{\omega}) \sim \mathbf{B}(\boldsymbol{\omega}) = \frac{K_d}{w}\,\mathbf{e}_\omega\mathbf{e}_\omega + O(1), \quad K_d = \begin{cases} 1 & \text{in 2-D,} \\ \dfrac{2}{\pi} & \text{in 3-D.} \end{cases} \tag{3.7c}$$

Note that K_d is a certain kind of a "stress-concentration" factor for the ellipsoidal cavity in the scalar conduction problem under discussion, in its degeneration into a crack.

The asymptotic formulae (3.7) will play a central role later on [Sections 5 and 6] when evaluating the appropriate coefficients in the variational estimate on the effective conductivity of the microcracked solid. Together with Lemma 2.1 and its Corollary 2.1 they allow us to show, in particular, that the field

$$U^{(1)}(\mathbf{x}) = \lim_{w\to 0} \int_\Omega T^{(1)}(\mathbf{x};\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega} \tag{3.8}$$

is finite everywhere in $\mathbb{R}^d$ $(d = 2, 3)$. The explicit form of $U^{(1)}(\mathbf{x})$ can be found by means of Lemma 2.1, but it will not be needed in the sequel.

4. THE VARIATIONAL PROCEDURE

Let $\kappa(\mathbf{x};\mathcal{S})$ be the conductivity field of the dispersion for a given realization $\mathcal{S} = \{\mathbf{x}_j, \boldsymbol{\omega}_j\}$ of spheroid centers and orientations. In the heat conduction context assume that the spheroids possess conductivity $\kappa_f = 0$ and the matrix κ_m, that is,

$$\kappa(\mathbf{x};\mathcal{S}) = \begin{cases} \kappa_m, & \text{if } \mathbf{x} \in \text{matrix,} \\ 0, & \text{if } \mathbf{x} \in \text{spheroids.} \end{cases} \tag{4.1}$$

With the aid of the random density field (2.8), this field admits a simple integral representation

$$\kappa(\mathbf{x};\mathcal{S}) = \kappa_m \left(1 - \int_{\mathbb{R}^d}\int_\Omega h(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}\right) = \langle\kappa(\mathbf{x};\mathcal{S})\rangle + \kappa'(\mathbf{x};\mathcal{S}),$$

where

$$\kappa'(\mathbf{x};\mathcal{S}) = -\kappa_m \int_{\mathbb{R}^d}\int_\Omega h(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega} \tag{4.2}$$

is the fluctuating part of the field $\kappa(\mathbf{x};\mathcal{S})$. Obviously,

$$\langle\kappa(\mathbf{x};\mathcal{S})\rangle = \kappa_m(1-nV_\omega) \to \kappa_m \quad \text{as} \quad w \to 0, \tag{4.3}$$

due to (2.9), where V_ω is the volume of a single spheroid and n denotes the number density of the spheroids. In (4.2), $\psi'(\mathbf{y};\boldsymbol{\omega}) = \psi(\mathbf{y};\boldsymbol{\omega}) - nP(\boldsymbol{\omega})$ is the fluctuating part of $\psi(\mathbf{y};\boldsymbol{\omega})$, so that $\langle\psi'(\mathbf{y};\boldsymbol{\omega})\rangle = 0$. [If not explicitly indicated, the integration hereafter with respect to spatial coordinates is over the whole $\mathbb{R}^d$, and that with respect to the "mark," i.e. spheroid's orientation, is over the unit sphere (or circle) Ω.]

The heat conduction through the dispersion is governed by the equations

$$\nabla\cdot(\kappa(\mathbf{x};\mathcal{S})\,\nabla\theta(\mathbf{x};\mathcal{S})) = 0, \quad \langle\nabla\theta(\mathbf{x};\mathcal{S})\rangle = \mathbf{G}, \tag{4.4}$$

where $\theta(\mathbf{x};\mathcal{S})$ is the random temperature field and $\mathbf{G}$ is the prescribed value of the macroscopically imposed temperature gradient. Then

$$\langle\kappa(\mathbf{x};\mathcal{S})\,\nabla\theta(\mathbf{x};\mathcal{S})\rangle = \kappa^*\mathbf{G}, \tag{4.5}$$

with κ^* denoting the effective conductivity of the dispersion and the brackets $\langle\cdot\rangle$ standing for ensemble averaging. It is emphasized however that the latter hereafter is over the set of all possible realizations of both locations and orientations of the spheroids.

Replace now (4.4) with the variational principle of classical type

$$\kappa^*G^2 \le W[\widetilde{\theta}(\cdot)], \quad W[\widetilde{\theta}(\cdot)] = \langle\kappa(\mathbf{x};\mathcal{S})\,|\nabla\widetilde{\theta}(\mathbf{x};\mathcal{S})|^2\rangle. \tag{4.6}$$

The functional W is considered over the class of fields with a prescribed mean gradient $\langle\nabla\widetilde{\theta}(\mathbf{x};\mathcal{S})\rangle = \mathbf{G}$. The minimum value of W is achieved on the actual temperature field $\theta(\mathbf{x};\mathcal{S})$ which solves the problem (4.4).

The proof of the variational principle (4.6) is entirely similar to the non-marked case when ensemble averaging is used [see Beran, 1968, and especially the reasoning in the footnote on pages 128, 129 there]. The only difference is that while the realizations in the non-marked case are point sets in $\mathbb{R}^3$, in the marked case they are again point sets, but in $\mathbb{R}^3\times\Omega$, which conceptually does not influence the reasoning at all. That is why the proof of the principle (4.6) will be omitted.

In the sequel a simple Ritz type procedure for the functional (4.6) will be employed, namely, trial fields of the form

$$\widetilde{\theta}(\mathbf{x};\mathcal{S}) = \mathbf{G}\cdot\mathbf{x} + \lambda\theta_1(\mathbf{x};\mathcal{S}) \tag{4.7}$$

will be chosen, where λ is an adjustable parameter, and $\theta_1(\mathbf{x};\mathcal{S})$ is fixed, with the only constraint that $\langle\theta_1(\mathbf{x};\mathcal{S})\rangle = 0$. Recall that the idea of using trial fields (4.7) for bounding the effective properties of heterogeneous solids was originated by Beran (1965), who additionally took θ_1 in a form suggested by the first-order term in the perturbation solution for a weakly inhomogeneous two-phase medium. In the context under discussion, this choice of Beran means that

$$\theta_1(\mathbf{x};\mathcal{S}) = \mathbf{G}\cdot\int\nabla G_0(\mathbf{x}-\mathbf{y})\kappa'(\mathbf{y};\mathcal{S})\,\mathrm{d}\mathbf{y}, \tag{4.8}$$

where $G_0(\mathbf{x})$ is the above mentioned Green function for the Laplace operator in $\mathbb{R}^d$. In the resulting bound [having optimized the functional (4.6) over the class (4.7) with respect to λ], the two- and three-point moments of the field $\kappa'(\mathbf{x},\boldsymbol{\omega})$ will enter, e.g., $M_2^\kappa(\mathbf{y}_1-\mathbf{y}_2) = \langle\kappa'(\mathbf{y}_1;\mathcal{S})\kappa'(\mathbf{y}_2;\mathcal{S})\rangle$, etc. However, a simple check using equations (4.2), (2.9) and Lemma 2.1 [more precisely, only the fact that

$$\int_\Omega h(\mathbf{x};\boldsymbol{\omega})\,P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega} = O(w)$$

as the aspect ratio $w \to 0$], demonstrates that $M_2^\kappa \to 0$ as $w \to 0$. The same conclusion holds true for the three- [and multi-] point moments of the field $\kappa'(\mathbf{x},\boldsymbol{\omega})$. This means that in the "crack" limit $w \to 0$ the conductivity field $\kappa(\mathbf{x};\mathcal{S})$ [see (4.1)] does not "feel" at all the presence of the cracks, i.e. it coincides, from a statistical point of view, just with the constant field κ_m, pertaining to a homogeneous matrix with no defects. In other words the trial fields (4.8) lose the information about the shape of the inclusion when $w \to 0$. As a consequence, the exact counterpart of the original Beran's bounds, corresponding here to the field $\theta_1(\mathbf{x})$ from (4.8), will yield for the microcracked solid the trivial upper bound κ_m.

The above result indicates that nontrivial bounds for the effective properties of cracked materials can be only obtained if one employs trial fields that retain information about the shape of the inclusions after taking the appropriate limit [$w \to 0$ in our case]. At least two classes of such trial fields can be immediately proposed. The first is a natural modification of the Beran choice (4.7)—(4.8). The second class will yield the so-called cluster bounds on the effective properties, which are of central interest in the present study. The common feature of both classes, as we shall see, is the replacement of the conductivity field $\kappa(\mathbf{x};\mathcal{S})$ by the random density field $\psi(\mathbf{x};\mathcal{S})$ in the right-hand side of (4.8), together with an appropriate change of the kernel function in the integrand there.

The first class of trial fields that leads to a nontrivial upper bound on the effective properties emerges if we divide the right-hand side of (4.8) by the aspect ratio w

$$\theta_1^{(b)}(\mathbf{x};\mathcal{S}) = \frac{1}{w}\,\mathbf{G}\cdot\int\nabla G_0(\mathbf{x}-\mathbf{y})\kappa'(\mathbf{y};\mathcal{S})\,\mathrm{d}\mathbf{y}.$$

Inserting here the representation (4.2) of $\kappa'(\mathbf{x};\mathcal{S})$ gives

$$\theta_1^{(b)}(\mathbf{x};\mathcal{S}) = \kappa_m\iint T^{(\mathrm{b})}(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\mathrm{d}\boldsymbol{\omega}, \tag{4.9}$$

where $\psi'(\mathbf{x};\boldsymbol{\omega}) = \psi(\mathbf{x};\boldsymbol{\omega}) - nP(\boldsymbol{\omega})$ is the already mentioned fluctuating part of $\psi(\mathbf{x};\boldsymbol{\omega})$, and

$$T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega}) = -\frac{1}{w}\,\mathbf{G}\cdot\nabla\varphi_\omega(\mathbf{x}). \tag{4.10}$$

It can be easily seen that in the "crack" limit $w \to 0$ the appropriate integrals containing the ratio $\nabla\varphi_\omega(\mathbf{x})/w$ do not degenerate. Also, the moments of the field $\psi'(\mathbf{y};\boldsymbol{\omega})$ depend on the statistics of the cracks' centers only. Thus optimizing, with respect to λ, the energy W over the class (4.7) at $\theta_1 = \theta_1^{(b)}$ produces a nontrivial upper bound, κ^b, on the effective conductivity, which can be called the modified Beran bound; accordingly, $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$ should be then called the modified Beran kernel. Due to reasons to be explained below, there is no need to examine κ^b in full detail.

It is now clear that other nontrivial bounds can be extracted from trial fields in the form (4.9) if one replaces $T^{(b)}(\mathbf{x};\boldsymbol{\omega})$ by any kernel with a similar to $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$ asymptotic behaviour in the "crack" limit. [The problem about the "best" such kernel is postponed until Section 6.] In particular, we can replace $T^{(b)}(\mathbf{x};\boldsymbol{\omega})$ by the single spheroid field $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$, discussed in Section 3, which possesses in the said limit the asymptotic form

$$T^{(1)}(\mathbf{x};\boldsymbol{\omega}) \sim -\frac{K_d}{w}\,\mathbf{G}\cdot\mathbf{e}_\omega\mathbf{e}_\omega\cdot\nabla\varphi_\omega(\mathbf{x}), \tag{4.11}$$

similar to (4.10), see (3.4) and (3.7). Hence instead of the Beran type choice (4.9), let us take in (4.7)

$$\theta_1(\mathbf{x};\mathcal{S}) = \theta_1^{(\mathrm{cl})}(\mathbf{x};\mathcal{S}) = \iint T^{(1)}(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}. \tag{4.12}$$

As a matter of fact the resulting bound will be just the so-called [first-order] cluster bound of Torquato (1986). The reason is clear, if one recalls the definition (2.8) of $\psi(\mathbf{y};\boldsymbol{\omega})$: the field $\theta_1^{(\mathrm{cl})}(\mathbf{x},\boldsymbol{\omega})$ represents a superposition of disturbances, introduced by the inclusions (spheroids) if each of them were alone in the unbounded matrix, subjected to constant temperature gradient at infinity. This interpretation indicates that the choice of the kernel as $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ is indeed most natural since for a dilute array of spheroids the temperature is a superposition of the single-spheroid fields, centered at the points $\mathbf{x}_j$. The adjustable parameter λ allows then to account, at least to a certain degree, for the mutual interaction of the spheroids when their concentration becomes higher.

As emphasized by Torquato (1986), the Beran and cluster bounds do not coincide in general, and their evaluations rely on different amounts of statistical information about the medium constitution. These bounds coincide only in certain special cases, e.g., for dispersions of nonoverlapping spheres (Torquato, 1986; Markov and Zvyatkov, 1987). [Torquato (1986) also noted that for some important random constitutions the cluster bounds are easier to be evaluated, say, for dispersions of overlapping spheres.] For microcracked solids the difference between the Beran and cluster bounds is even more striking: While the former degenerates for such solids, as already demonstrated, the latter provides a nontrivial upper bound on the effective conductivity under study [Section 5]. Even the modified Beran bound [corresponding to the kernel (4.10)], though nontrivial in the "crack" limit, is inferior to the cluster one, as we shall see below.

It is remarked that trial fields of the "cluster type" (4.12) seem to have first been used by Weissberg (1963) in the context of diffusion in a porous solid. A similar idea for bounding the elastic moduli of cracked bodies [fiber composites, to be precise] was used, perhaps for the first time, by Gottesman *et al.* (1980) but without optimizing with respect to λ. The authors just took $\lambda = 1$ and evaluated the elastic energy for the superposition of the single crack fields in the composite [see their equation (3.3), p. 753], which lead to fairly simple estimates on the needed moduli. As we shall see, this intuitive choice of λ turns out to be very appropriate, due to reasons which will be discussed later [Section 5].

It is important to emphasize also that introducing the fluctuating part $\psi'(\mathbf{x};\boldsymbol{\omega})$ in (4.12), instead of the field $\psi(\mathbf{x};\boldsymbol{\omega})$ itself, is important from a formal point of view, since in this way all the integrals that appear in the sequel are absolutely convergent and thus there is no need for a [tacit or explicit] "renormalization" of conditionally convergent integrals.

Now, to evaluate the cluster bounds, (4.12) and (4.7) should be inserted into the energy (4.6), thus turning the latter into a quadratic function of λ

$$W = W(\lambda) = \kappa_m(A - 2B\lambda + C\lambda^2), \tag{4.13a}$$

with the coefficients

$$A = G^2\langle\kappa\rangle/\kappa_m,$$

$$B = \mathbf{G}\cdot\iiint h(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1)\,\nabla T^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2)\langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2,$$

$$\begin{aligned} C = &\iiint \nabla T^{(1)}(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1)\cdot\nabla T^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2)\langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2 \\ &- \iiint h(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1)\,\nabla T^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2)\cdot\nabla T^{(1)}(\mathbf{x}-\mathbf{y}_3;\boldsymbol{\omega}_3) \\ &\quad\times\langle\psi(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\psi'(\mathbf{y}_3;\boldsymbol{\omega}_3)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\mathrm{d}\mathbf{y}_3\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2\mathrm{d}\boldsymbol{\omega}_3, \end{aligned} \tag{4.13b}$$

since $\langle\psi(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle = \langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle$.

Minimizing the quadratic function in (4.13a) and taking the "crack" limit $w = c/a \to 0$ yields the estimate

$$\kappa^* \le \kappa^{\mathrm{cl}}, \quad \kappa^{\mathrm{cl}} = \kappa_m\left(\lim_{w\to 0} A - \frac{\left[\lim\limits_{w\to 0} B\right]^2}{\lim\limits_{w\to 0} C}\right) \Big/ G^2. \tag{4.14}$$

This will be exactly the first-order cluster bound of Torquato for the microcracked solid under study. The estimate (4.14) is obviously three-point in the sense that it depends on the k-point probability densities f_k for the set of cracks' centers up to $k = 3$.

To find the bound (4.14) explicitly the problems to be overcome become now purely technical: Making use of the formulae (2.9) for the moments of the random density field and the results of Sections 2 and 3, one should evaluate the coefficients A, B and C from (4.13b) for a given spatial statistics in the aforementioned "crack" limit $w = c/a \to 0$. The eventual result will be reported in the next section.

It is to be pointed out that the very form of the trial fields (4.12) suggests an obvious generalization, namely, to take the kernel $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ adjustable, instead of fixing it as the single-spheroid field. In this way, the "best" three-point bound, obtainable within such a broader class of trial fields can be derived. This idea will be treated in more details in Section 6. However, it is convenient to consider first in detail the particular case (4.12), since the intermediate calculations and remarks will prove useful and serve as a lead in this more general situation.

5. THE CLUSTER BOUND IN THE SCALAR CASE

First, as it follows from (4.13b) and (4.3),

$$A_0 = \lim_{w\to 0} A = G^2. \tag{5.1}$$

To evaluate B, note that

$$\langle \psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle = nP(\boldsymbol{\omega}_1)\delta(\mathbf{y}_{1,2})\delta(\boldsymbol{\omega}_{1,2}) - n^2 P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)R(\mathbf{y}_{1,2}), \tag{5.2}$$

as a consequence of (2.9), where

$$R(\mathbf{y}) = 1 - g(\mathbf{y}), \quad g(\mathbf{y}) = f_2(0,\mathbf{y})/n^2, \tag{5.3}$$

so that $g(\mathbf{y})$ is just the radial distribution function for the spheroids' centers and hence $-R(\mathbf{y})$ is the so-called binary [or total] correlation function, often denoted as $\nu_2(\mathbf{y})$ in the liquid state theory. Inserting (5.2) into the formula for B [see (4.13b)] gives

$$B = nB_1 - n^2 B_2, \tag{5.4}$$

with the coefficients

$$B_1 = \mathbf{G}\cdot\iint h(\mathbf{z};\boldsymbol{\omega})\,\nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\mathbf{z}\,\mathrm{d}\boldsymbol{\omega}, \tag{5.5a}$$

$$B_2 = \mathbf{G}\cdot\iiiint h(\mathbf{z}_1;\boldsymbol{\omega}_1)\,\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)R(\mathbf{z}_1-\mathbf{z}_2)\,P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)\,\mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2, \tag{5.5b}$$

having made obvious changes of variables in the integrals.

The evaluation of the coefficient B_1 can be done by means of Corollary 2.1, but it is even simpler if one employs (3.2): $h(\mathbf{x};\boldsymbol{\omega})\nabla T^{(1)}(\mathbf{x};\boldsymbol{\omega}) = h(\mathbf{x};\boldsymbol{\omega})\mathbf{B}(\boldsymbol{\omega})\cdot\mathbf{G}$, so that

$$B_1 = V_\omega \mathbf{G}\cdot\int_\Omega \mathbf{B}(\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega}\cdot\mathbf{G}. \tag{5.6}$$

The tensor

$$\int_\Omega \mathbf{B}(\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega}$$

is isotropic; using the asymptotic formulae (3.7) of $\mathbf{B}(\boldsymbol{\omega})$ in the "crack" limit $w\to 0$, we have

$$\int_\Omega \mathbf{B}(\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega} = \frac{K_d}{wd}\,\mathbf{I} + O(1) \quad \text{as} \quad w\to 0.$$

Hence, in virtue of (3.7b) and (5.6),

$$\lim_{w\to 0} B_1 = \frac{K_d}{d}\,V_a G^2 = G^2 \begin{cases} \dfrac{1}{2}\pi a^2 & \text{in 2-D,} \\ \dfrac{8}{9}\,a^3 & \text{in 3-D.} \end{cases} \tag{5.7}$$

In turn, the coefficient B_2 in the "crack" limit vanishes, since it can be recast as

$$\lim_{w\to 0} B_2 = \mathbf{G}\cdot\iint \nabla U^{(1)}(\mathbf{z}_2)\left[\lim_{w\to 0}\int_\Omega h(\mathbf{z}_1;\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_1)\,\mathrm{d}\boldsymbol{\omega}_1\right] R(\mathbf{z}_1-\mathbf{z}_2)\,\mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2 = 0, \tag{5.8}$$

with $U^{(1)}(\mathbf{x})$ given in (3.8); the reason is that the function $U^{(1)}(\mathbf{x})$ is finite everywhere, as already pointed out, and $R(\mathbf{z}_1-\mathbf{z}_2)$ does not depend on w, while the term in the square brackets in (5.8) vanishes in the limit $w\to 0$ [see (2.10a)].

To evaluate the coefficient C from (4.13b), note first that

$$\begin{aligned}\langle\psi(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\psi'(\mathbf{y}_3;\boldsymbol{\omega}_3)\rangle &= nP(\boldsymbol{\omega}_1)\delta(\mathbf{y}_{1,2})\delta(\mathbf{y}_{1,3})\delta(\boldsymbol{\omega}_{1,2})\delta(\boldsymbol{\omega}_{1,3})\\ -\,n^2\,3\{P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)R(\mathbf{y}_{1,2})\delta(\mathbf{y}_{1,3})\delta(\boldsymbol{\omega}_{1,3})\}_s &+ n^2\,P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)\delta(\mathbf{y}_{2,3})\delta(\boldsymbol{\omega}_{2,3})\\ &+ n^3P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)P(\boldsymbol{\omega}_3)G_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3),\end{aligned} \tag{5.9}$$

with

$$G_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3) = g_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3) - 1 + R(\mathbf{y}_{1,2}) + R(\mathbf{y}_{1,3}), \tag{5.10}$$

which again simply follows from (2.9); recall that $\{\cdot\}_s$ means symmetrization with respect to the indices in the braces [in our case $\{1,2,3\}$]. In (5.10), $g_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3) = f_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)/n^3$ is the three-point counterpart of the radial distribution function $g(r)$ [see (5.3)]. As a consequence of the no long-range order hypothesis in the crack's spatial location, $G_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)\to 0$ when all distances between the points $\mathbf{y}_1$, $\mathbf{y}_2$ and $\mathbf{y}_3$ go to infinity.

Inserting now (5.2) and (5.9) into the formula (4.13b) for C gives

$$C = nC_1 - n^2C_2 - n^3C_3, \tag{5.11}$$

$$C_1 = C_{11} - C_{12}, \quad C_2 = C_{21} - C_{22} + C_{23}, \quad C_{22} = 2C'_{22} + C''_{22}. \tag{5.12}$$

Appendix A contains the explicit forms of the coefficients C's in (5.11) and (5.12) and details of their evaluation. The eventual result reads

$$\lim_{w\to 0} B = B_0, \quad C_0 = \lim_{w\to 0} C = B_0(1+B_0), \quad B_0 = \frac{K_d}{d}\,\alpha_d, \tag{5.13}$$

where the value of B_0 follows from (5.4), (5.7) and (5.8). Hence the "best" cluster kernel, $T^{\mathrm{cl}}(\mathbf{x};\boldsymbol{\omega})$, in the class (4.7), (4.12) is

$$T^{\mathrm{cl}}(\mathbf{x};\boldsymbol{\omega}) = \lambda_0 T^{(1)}(\mathbf{x};\boldsymbol{\omega}), \quad \lambda_0 = \frac{B_0}{C_0} = \frac{1}{1+B_0}\,. \tag{5.14}$$

With the values of B and C in the "crack" limit [see (5.1) and (5.13)], the cluster bound (4.14) on the effective conductivity of the microcracked solid under study becomes

$$\frac{\kappa^{\mathrm{cl}}}{\kappa_m} = \frac{1}{1+\dfrac{K_d}{d}\,\alpha_d} = \begin{cases} \dfrac{1}{1+\frac{8}{9}\,na^3} & \text{in 3-D,}\\[2ex] \dfrac{1}{1+\frac{1}{2}\,\pi na^2} & \text{in 2-D,}\end{cases} \tag{5.15}$$

where $\alpha_d = nV_a$ is the dimensionless crack "fraction" in the body, as already introduced in (2.5), i.e. $\alpha_2 = \pi\varepsilon$ in 2-D and $\alpha_3 = \frac{4}{3}\pi\varepsilon$ in 3-D; ε is the often used crack concentration measure [na^2 or na^3 in 2-D and 3-D respectively, see Kachanov (1992)].

The cluster bound (5.15) admits a simple and important interpretation. Namely, imagine that each spheroid is isolated and embedded into the constant flux field $\mathbf{q} = \mathbf{G}/\kappa_m$. Then the effective "compliance," $1/\kappa^*$, of the solid is a linear function of the spheroids' density n, since their mutual interactions are neglected. Summing appropriately the contributions from each spheroid, averaging over orientation and taking the "crack" limit reproduces the cluster bound (5.15). Thus the latter exactly corresponds to the well-known approximation, called by Kachanov (1992) "approximation of non-interacting cracks." The same coincidence will be noticed and discussed in the elastic case as well [Section 8].

Note that one can directly take $\lambda = 1$ in (4.7), without optimizing the right-hand side of (4.13a). This yields the upper bound

$$\frac{\kappa^{\mathrm{up}}}{\kappa_m} = 1 - 2B_0 + C_0 = 1 - \frac{K_d}{d}\,\alpha_d + \left(\frac{K_d}{d}\right)^2 \alpha_d^2. \tag{5.16}$$

The bound (5.16) is very close to the cluster one (5.15) and the difference between them is less than 1.5 % at $\alpha_d \leq 0.6$. The reason is that for these values of α_d, the optimal multiplier λ_0 in (4.12) is very close to 1 [see (3.7c), (5.13) and (5.14)]. It is the scalar conductivity counterpart of the above mentioned bounds of Gottesman *et al.* (1980) for the elastic moduli of a fiber-reinforced material, because at $\lambda = 1$ the trial field (4.7), (4.12) represents a superposition of the single [isolated] crack fields $T^{(1)}(\mathbf{x} - \mathbf{x}_j; \boldsymbol{\omega}_j)$, located at the crack centers $\mathbf{x}_j$, plus the field $\widetilde{\mathbf{G}} \cdot \mathbf{x}$ with a certain constant gradient $\widetilde{\mathbf{G}}$ [in order to satisfy the condition (4.4) of prescribed macroscopic gradient]. However, use of such a trial field in the variational principle (4.12) would give rise to conditionally convergent integrals; the latter are avoided here, let us point out once again, by using the fluctuating part $\psi'(\mathbf{x}; \boldsymbol{\omega})$ of the random density field (2.8), instead of $\psi(\mathbf{x}; \boldsymbol{\omega})$ itself, in the representation (4.12).

It is to be also observed that the bound κ^{up} coincides formally with the quadratic approximation in crack density α_d of the cluster bound (5.15). Since $\kappa^{\mathrm{cl}} \leq \kappa^{\mathrm{up}}$, the fact that κ^{up} represents a bound is trivial. We have mentioned it only because it corresponds to the above discussed special choice of trial fields at $\lambda = 1$.

It is important to point out the close resemblance between (5.15) and the bound derived by Willis (1977). Namely, Willis considered a matrix containing a family of identical and aligned spheroids, all of them perpendicular to an axis Ox_1, and then applied appropriately the Hashin-Shtrikman variational principle. When the spheroids are voids and degenerate into penny-shaped cracks of density α_d, the result of Willis was the estimate

$$\frac{\kappa_{11}^*}{\kappa_m} \leq \frac{1}{1 + K_d\,\alpha_d} \tag{5.17}$$

for the effective conductivity component κ_{11}^* of the solid along the axis Ox_1. [The estimate (5.17) was rederived by Torquato and Lado, 1991, using different arguments.] Formally, the cluster bound (5.15) "follows" from (5.17) if a special microstructure of cracks' distribution is assumed. Indeed, consider a solid containing three [in 3-D or two in 2-D] mutually orthogonal families of penny-shaped cracks, whose opening vectors are along the axes Ox_i $(i = 1, \ldots, d)$

of given Cartesian system. Each crack family is statistically homogeneous with density α_d/d. Such a microcracked solid is obviously macroscopically isotropic as far as its heat conduction properties are considered. In the case under study

$$\kappa^* = \kappa^*_{11} = \kappa^*_{22} = \kappa^*_{33} \ \text{ in 3-D} \quad \text{or} \quad \kappa^* = \kappa^*_{11} = \kappa^*_{22} \ \text{ in 2-D}, \tag{5.18}$$

since the effective conductivity is affected only by the cracks perpendicular to the applied microscopic temperature gradient $\mathbf{G}$, and each family has one and the same crack density α_d/d. Then (5.18) and (5.17) [with α_d replaced by α_d/d] imply the cluster bound (5.15).

The foregoing reasoning clearly indicates that though the bound (5.15) closely resembles the bound of Willis (5.17), they pertain to different kinds of cracks' statistics. Indeed, (5.15) is inherently connected with the fundamental assumption (2.2) and (2.3) of non-correlated location and orientation in the cracks' assemblage. At the same time the bound (5.17) requires aligned systems of microcracks or an appropriate assemblage of such systems in order to reproduce (5.15).

A remark concerning the above mentioned [Section 4] modified Beran bound, κ^b, is finally warranted. Its evaluation can be performed in a manner, entirely similar to that of the cluster one, upon replacing the kernel $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ by the kernel $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$, as given in (4.10). The bound κ^b is evaluated in the dilute case in Appendix B. It turns out that even in this case it is worse than the cluster bound and, unlike the latter, fails to reproduce the exact α_d-coefficient of the effective conductivity, underestimating it twice. But this is fully natural, since in the dilute case, when the cracks' interactions are negligible, the appropriate kernel in the class (4.9) should be indeed the single-spheroid field $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$; any other field, in particular, $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$, would produce results, incorrect even in this simplest case.

6. ON THE "OPTIMIZED" CLUSTER BOUND IN THE SCALAR CASE

As already mentioned, one can try improving the cluster bound, if instead of the class (4.7), (4.12), the more general class of trial fields is introduced, namely,

$$\theta(\mathbf{x};\mathcal{S}) = \mathbf{G}\cdot\mathbf{x} + \lambda\iint T(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}, \tag{6.1}$$

with both λ and $T(\mathbf{x};\boldsymbol{\omega})$ adjustable. Of course, it suffices to take $\lambda = 1$ in (6.1), but it will prove useful later to allow both quantities to vary independently. The upper bound on the effective conductivity of the microcracked solid that follows from minimizing the energy (4.12) over the class (6.1) [in the "crack" limit $w = c/a \to 0$] is denoted by $\widetilde{\kappa}$, i.e.

$$\kappa^* \le \widetilde{\kappa}, \quad \widetilde{\kappa}\,G^2 = \lim_{w\to 0}\ \min_{\lambda,\,T(\cdot)} W,$$

and will be referred to as the optimized cluster-type bound. The reason is clear: the trial fields (6.1) represent, similarly to (4.1), a superposition of the fields $T(\mathbf{x}-\mathbf{x}_i;\boldsymbol{\omega}_i)$, "centered" at the crack locations $\mathbf{x}_i$. However, the "disturbance" $T(\mathbf{x};\boldsymbol{\omega})$ is now adjustable, feeling the presence of the rest of the cracks. Note that a similar class of trial fields was first introduced,

to the best of the author's knowledge, by Prager (1963) in his study of variational bounds on the effective behaviour of dispersions of spheres in a scalar context, where he derived an integral equation for the "best" kernel $T(\mathbf{x})$. [For further development see also Markov and Zvyatkov (1991) and the references therein.]

The restriction of the energy functional W [see (4.12)] over the class (6.1) has the quadratic form (4.13a) with respect to λ

$$W = W[\lambda, T(\cdot)] = \kappa_m(A - 2B\lambda + C\lambda^2), \tag{6.2}$$

with the same A [see (4.13a)], and with the coefficients B and C of the form, given in the same equation (4.13b). The important difference is that the fixed single-spheroid field $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ is everywhere replaced there by the adjustable kernel $T(\mathbf{x};\boldsymbol{\omega})$, so that $B = B[T(\cdot)]$ and $C = C[T(\cdot)]$ are known functionals of this kernel, depending in an explicit manner on the two and three-point cracks' statistics.

To get a simpler formula for the cluster-type bound $\widetilde{\kappa}^*$, let us minimize (6.2) in two different ways. First, at fixed $T(\mathbf{x};\boldsymbol{\omega})$, minimize it with respect to λ:

$$\min_{\lambda} W \le \kappa_m \left(A - \frac{B^2}{C} \right),$$

and then minimize the right-hand side of the latter with respect to $T(\mathbf{x};\boldsymbol{\omega})$

$$\widetilde{\kappa} G^2 = \min_{\lambda,\, T(\cdot)} W \le \kappa_m \left(A - \max_{T(\cdot)} \frac{B^2}{C} \right). \tag{6.3}$$

But this is equivalent to minimizing (6.2) with respect to the kernel $T(\mathbf{x};\boldsymbol{\omega})$ at $\lambda = 1$:

$$\widetilde{\kappa} G^2 = \min_{\lambda=1,\, T(\cdot)} W \le \kappa_m \left[A - \max_{T(\cdot)} (2B - C) \right]. \tag{6.4}$$

The functionals B^2/C and $2B - C$ are maximized at one and the same kernel $T(\mathbf{x};\boldsymbol{\omega})$—the optimal one which brings forth the best possible bound, $\widetilde{\kappa}$, on the effective conductivity, derivable from the class (6.1). This optimal kernel will be denoted in the sequel as $\widetilde{T}(\mathbf{x};\boldsymbol{\omega})$. Moreover, the maximum values of these two functionals coincide, that is

$$\frac{B^2[\widetilde{T}(\cdot)]}{C[\widetilde{T}(\cdot)]} = 2\, B[\widetilde{T}(\cdot)] - C[\widetilde{T}(\cdot)],$$

which immediately yields

$$B[\widetilde{T}(\cdot)] = C[\widetilde{T}(\cdot)]. \tag{6.5}$$

Hence, as it follows from (6.3) or (6.4),

$$\widetilde{\kappa}\, G^2 = \kappa_m \lim_{w \to 0} \big(A - B[\widetilde{T}(\cdot)] \big). \tag{6.6}$$

In turn, the functional $B[T(\cdot)]$, according to (4.13b) and (5.2), can be recast as

$$B[T(\cdot)] = n\mathbf{G} \cdot \iint H(\mathbf{x};\boldsymbol{\omega}) \nabla T(\mathbf{x};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{x}\mathrm{d}\boldsymbol{\omega}$$

$$= n\mathbf{G} \cdot \iint h(\mathbf{x};\boldsymbol{\omega}) \nabla S(\mathbf{x};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{x}\mathrm{d}\boldsymbol{\omega}, \tag{6.7}$$

where

$$S(\mathbf{x};\boldsymbol{\omega}) = \mathcal{R}\,[T]\,(\mathbf{x};\boldsymbol{\omega}), \quad H(\mathbf{x};\boldsymbol{\omega}) = \mathcal{R}\,[h]\,(\mathbf{x};\boldsymbol{\omega}), \tag{6.8}$$

and $\mathcal{R}$ denotes the integral operator acting on the functions $u(\mathbf{x};\boldsymbol{\omega})$ over $\mathbb{R}^d \times \Omega$ as

$$\mathcal{R}\,[u](\mathbf{x};\boldsymbol{\omega}) = u(\mathbf{x};\boldsymbol{\omega}) - n \iint R(\mathbf{x}-\mathbf{y})\, u(\mathbf{y};\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_1)\, \mathrm{d}\mathbf{y}\mathrm{d}\boldsymbol{\omega}_1. \tag{6.9}$$

By means of the operator $\mathcal{R}$ the optimized bound (6.6) can be recast as

$$\widetilde{\kappa}\, G^2 = \kappa_m \lim_{w\to 0} \left(A - n \iint H(\mathbf{x};\boldsymbol{\omega}) \nabla \widetilde{T}(\mathbf{x};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{x}\mathrm{d}\boldsymbol{\omega} \right), \tag{6.10}$$

with $H(\mathbf{x};\boldsymbol{\omega})$ defined in (6.8). Note that the very form (6.8) of this function suggests that the bound $\widetilde{\kappa}$ is nontrivial only if the kernel $\widetilde{T}(\mathbf{x};\boldsymbol{\omega})$ has in the "crack" limit the following asymptotic behaviour

$$\widetilde{T}(\mathbf{x};\boldsymbol{\omega}) = \frac{\text{const}}{w} + O(1) \quad \text{as} \quad w \to 0. \tag{6.11}$$

Since the leading term in the asymptotic expansion of the single-spheroid field $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$ is also $1/w$ [see (3.4) and (3.7)], this implies that the optimal kernel can be sought, for example, in the form

$$\widetilde{T}(\mathbf{x};\boldsymbol{\omega}) = \lambda T^{(1)}(\mathbf{x};\boldsymbol{\omega}) + \Phi(\mathbf{x};\boldsymbol{\omega}), \tag{6.12}$$

where both the scalar λ and the function $\Phi(\mathbf{x};\boldsymbol{\omega})$ are adjustable; moreover, $\Phi(\mathbf{x};\boldsymbol{\omega})$ is independent of the aspect ratio w. [More precisely, the "regular" part $\Phi(\mathbf{x};\boldsymbol{\omega})$ of the kernel $\widetilde{T}(\mathbf{x};\boldsymbol{\omega})$ should remain finite in the limit $w \to 0$ and since we are interested only in what remains after taking this limit, we can indeed assume $\Phi(\mathbf{x};\boldsymbol{\omega})$ independent of w already in this stage of the analysis.] As a consequence, all integrals containing $\Phi(\mathbf{x};\boldsymbol{\omega})$ and the characteristic function $h(\mathbf{x};\boldsymbol{\omega})$ disappear in the "crack" limit. This drastically simplifies the form of the energy functional W [see (4.13)], when restricted over the class (6.12), namely,

$$W = W[\lambda;\Phi(\cdot)] = \kappa_m(A - 2B\lambda + C\lambda^2) + \mathcal{F}[\lambda;\Phi(\cdot)], \tag{6.13}$$

with the same coefficients A, B, C as in (5.13), and

$$\mathcal{F}[\lambda;\Phi(\cdot)] = \left\langle \left| \iint \nabla\Phi(\mathbf{x};\boldsymbol{\omega}) \psi'(\mathbf{x};\boldsymbol{\omega})\, \mathrm{d}\mathbf{x}\mathrm{d}\boldsymbol{\omega} \right|^2 \right\rangle + 2\lambda \mathcal{F}_1[\lambda;\Phi(\cdot)], \tag{6.14}$$

where

$$\begin{aligned}\mathcal{F}_1[\Phi(\cdot)] = &\iiiint \nabla T^{(1)}(\mathbf{y}_1;\boldsymbol{\omega}_1) \cdot \nabla\Phi(\mathbf{y}_2;\boldsymbol{\omega}_2) \langle \psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\, \mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2 \\ &- \iiiiiint h(\mathbf{y}_1;\boldsymbol{\omega}_1) \nabla T^{(1)}(\mathbf{y}_2;\boldsymbol{\omega}_2) \cdot \nabla\Phi(\mathbf{y}_3;\boldsymbol{\omega}_3) \\ &\times \langle \psi(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\psi'(\mathbf{y}_3;\boldsymbol{\omega}_3)\rangle\, \mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\mathrm{d}\mathbf{y}_3\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2\mathrm{d}\boldsymbol{\omega}_3. \end{aligned} \tag{6.15}$$

It is clear that only the terms for which $\mathbf{y}_1 = \mathbf{y}_2$ will not vanish in the six-fold integral in (6.15), i.e. we should keep only the terms containing $\delta(\mathbf{y}_1 - \mathbf{y}_2)$ in the formula (5.9).

What remains from the latter is just the two-point moment $\langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle$, so that the functional $\mathcal{F}_1[\lambda;\Phi(\cdot)]$, defined in (6.15), can be written as

$$\mathcal{F}_1[\Phi(\cdot)] = \iiint [1 - h(\mathbf{y}_1;\boldsymbol{\omega}_1)]\,\nabla T^{(1)}(\mathbf{y}_1;\boldsymbol{\omega}_1)\cdot\nabla\Phi(\mathbf{y}_2;\boldsymbol{\omega}_2)$$

$$\times\,\langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2. \tag{6.16}$$

The two-point moment $\langle\psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle$ contains a singular part, proportional to $\delta(\mathbf{y}_1-\mathbf{y}_2)\delta(\boldsymbol{\omega}_1-\boldsymbol{\omega}_2)$, and a regular part that depends on $\mathbf{y}_1-\mathbf{y}_2$ only [see (5.2)]. Consequently, an obvious integration by parts in (6.16) allows $\mathcal{F}_1[\Phi(\cdot)]$ to be recast in an integral form with an integrand, containing the factor

$$\Delta T^{(1)}(\mathbf{y}_1;\boldsymbol{\omega}_1) - \nabla\cdot\Big(h(\mathbf{y}_1;\boldsymbol{\omega}_1)\nabla T^{(1)}(\mathbf{y}_1;\boldsymbol{\omega}_1)\Big). \tag{6.17}$$

This factor vanishes in the "crack" limit, as it follows from (3.2) at $\kappa_f = 0$. Hence, the additional term in the energy W, introduced by the adjustable kernel $\Phi(\mathbf{x};\boldsymbol{\omega})$, is

$$\mathcal{F}[\lambda;\Phi(\cdot)] = \left\langle \left| \iint \nabla\Phi(\mathbf{x};\boldsymbol{\omega})\psi'(\mathbf{x};\boldsymbol{\omega})\,\mathrm{d}\mathbf{x}\mathrm{d}\boldsymbol{\omega} \right|^2 \right\rangle \geq 0$$

[see (6.13)] and therefore it does not depend on λ, being always nonnegative. From (6.13) it then follows that $\lambda = B/C$ and $\Phi(\mathbf{x};\boldsymbol{\omega}) \equiv 0$ minimize the energy W. But, as already pointed out, the coefficients A, B and C are the same as in (5.13) which means that the cluster bound (5.15) cannot be improved for a microcracked solid, if the much broader class (6.12) of trial fields is employed instead of (4.7) and (4.12).

It is important to point out that the latter result does not yet imply that the cluster bound (5.15) coincides with the optimal one, $\widetilde{\kappa}$, and hence the problem of evaluating $\widetilde{\kappa}$ for the microcracked solid remains open. The reason lies in the fact that (6.11) does not yield that the singular part of the optimal kernel is proportional to $T^{(1)}(\mathbf{x};\boldsymbol{\omega})$. For example, the modified Beran kernel $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$ [see (4.10)] has the same asymptotic form (6.11) as $w \to 0$. One can therefore repeat the foregoing reasoning literally, replacing the class (6.12) of trial fields by the class $\lambda T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega}) + \Phi(\mathbf{x};\boldsymbol{\omega})$. The factor (6.17) in this case does not vanish, however, containing a singular part whose support is the surface of the spheroid S_ω. Hence $\mathcal{F}_1[\Phi(\cdot)]$ does not vanish either and one cannot claim as a result that $\Phi(\mathbf{x};\boldsymbol{\omega}) = 0$ is the best choice. The modified Beran bound κ^b can be therefore improved upon adding an appropriate "regular" part $\Phi(\mathbf{x};\boldsymbol{\omega})$ to the kernel $T^{(\mathrm{b})}(\mathbf{x};\boldsymbol{\omega})$. In view of the fact that κ^b is worse than the cluster bound even in the dilute case [see Appendix B], this conclusion should not be a surprise however.

7. THE ELASTIC CASE

Consider an isotropic elastic matrix with tensor of elastic moduli

$$\mathbb{L}_m = k_m\,\mathbb{J}' + 2\mu_m\,\mathbb{J}'', \tag{7.1}$$

where $\mathbb{J}'$ and $\mathbb{J}''$ are the two basic isotropic fourth-rank tensors with the components

$$J'_{ijkl} = \delta_{ij}\delta_{kl}, \quad J''_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}\right); \tag{7.2}$$

$k_m = \lambda_m + \frac{2}{3}\,\mu_m$ is the bulk modulus.

Let the matrix contain an isotropic spheroidal elastic inhomogeneity S_ω with elastic moduli κ_f and μ_f. The notations of Section 2 will be used afterward, in particular, the axis x_3 is again along the shortest semiaxis of the spheroid. Denote by $\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})$ the disturbance to the displacement field, introduced by the inhomogeneity within the unbounded matrix, provided the strain tensor at infinity equals $\mathbf{E}$ [a prescribed constant second-rank symmetric tensor]. As is well-known, the strain tensor in the inhomogeneity is then also constant; moreover

$$\boldsymbol{\varepsilon}^{(1)}(\mathbf{x};\boldsymbol{\omega}) = \mathbb{B}(\boldsymbol{\omega}) : \mathbf{E}\,, \quad \mathbf{x} \in S_\omega. \tag{7.3}$$

Here

$$\boldsymbol{\varepsilon}^{(1)}(\mathbf{x};\boldsymbol{\omega}) = \operatorname{def}\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega}) = \tfrac{1}{2}\,(\,\nabla\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega}) + \Big(\nabla\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})\Big)^T\,)$$

is the [small] strain tensor associated with the displacement $\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})$, the colon standing for contraction with respect to two pairs of indices. The field $\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})$ solves an equation, similar to (3.1). Hereafter only the case of a spheroidal cavity [$k_f = \mu_f = 0$] will be dealt with for which this equation can be recast as

$$\nabla\cdot\Big(\mathbb{L}_m : \nabla\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})\Big) - \nabla\cdot\Big(h(\mathbf{x};\boldsymbol{\omega})\mathbb{L}_m : (\mathbb{B}(\boldsymbol{\omega}) + \mathbb{J}) : \mathbf{E}\Big) = 0 \tag{7.4}$$

—having used (7.3) and the symmetry properties of the elastic tensor $\mathbb{L}_m$; in (7.4) $\mathbb{J}$ denotes the unit fourth-rank tensor.

The notations of Hill (1963a) are not so useful here in this particular situation as they are for a general transversely isotropic symmetry], and it is better to write the fourth-rank tensor $\mathbb{B}(\boldsymbol{\omega})$ in a direct polyadic form, for the case of a spheroidal cavity under study, and keeping only the leading term in its asymptotic in the "crack" limit $w \to 0$:

$$\begin{aligned}\mathbb{B}(\boldsymbol{\omega}) = \frac{4}{\pi w}\Big\{&\mathbf{e}_3\mathbf{e}_3\Big[\,E'(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2) + E''\mathbf{e}_3\mathbf{e}_3\,\Big] \\ &+ E'''\Big[\,\mathbf{e}_{(1}\mathbf{e}_{3)}\,\mathbf{e}_{(1}\mathbf{e}_{3)} + \mathbf{e}_{(2}\mathbf{e}_{3)}\,\mathbf{e}_{(2}\mathbf{e}_{3)}\,\Big]\Big\} + O(1),\end{aligned} \tag{7.5a}$$

where $\mathbf{e}_{(i}\mathbf{e}_{j)} = \frac{1}{2}(\mathbf{e}_i\mathbf{e}_j + \mathbf{e}_j\mathbf{e}_i)$. The coefficients in (7.5a) depend on the Poisson ratio ν_m of the matrix only, namely,

$$E' = \frac{\nu_m(1-\nu_m)}{1-2\nu_m}\,, \quad E'' = \frac{(1-\nu_m)^2}{1-2\nu_m}\,, \quad E''' = \frac{1-\nu_m}{2-\nu_m}\,. \tag{7.5b}$$

The formulae (7.5) can be extracted from the appropriate results collected and comprehensively discussed in the book of Mura (1988).

It is noted that the tensor $\mathbb{B}(\boldsymbol{\omega})$, averaged over all orientations $\boldsymbol{\omega}$, is isotropic and hence it has the form (7.1),

$$\overline{\mathbb{B}} = \int_\Omega \mathbb{B}(\boldsymbol{\omega})P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega} = \frac{1}{w}\,\overline{\mathbb{B}}^{\,\omega} + O(1)\,, \quad \overline{\mathbb{B}}^{\,\omega} = \lim_{w\to 0} w\overline{\mathbb{B}},$$

$$\overline{\mathbb{B}}^{\omega} = \overline{k}^{\omega}\,\mathbb{J}' + 2\overline{\mu}^{\omega}\,\mathbb{J}''. \tag{7.6a}$$

The coefficients $\overline{k}^{\omega}$ and $\overline{\mu}^{\omega}$ can be easily found from (7.5):

$$\overline{k}^{\omega} = \frac{4}{3\pi}\,\frac{1-\nu_m^2}{1-2\nu_m}\,, \quad \overline{\mu}^{\omega} = \frac{4}{15\pi}\,\frac{(1-\nu_m)(5-\nu_m)}{2-\nu_m}\,. \tag{7.6b}$$

The elastic moduli field of the dispersion has the form

$$\mathbb{L}(\mathbf{x};\mathcal{S}) = k(\mathbf{x};\mathcal{S})\,\mathbb{J}' + 2\mu(\mathbf{x};\mathcal{S})\,\mathbb{J}'', \tag{7.7}$$

where

$$k(\mathbf{x};\mathcal{S}) = k_m\left(1 - \int_{\mathbb{R}^3}\int_{\Omega} h(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}\right), \tag{7.8a}$$

$$\mu(\mathbf{x};\mathcal{S}) = \mu_m\left(1 - \int_{\mathbb{R}^3}\int_{\Omega} h(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}\right). \tag{7.8b}$$

Moreover, similarly to (4.3), one has in the "crack" limit $w \to 0$,

$$\langle k(\mathbf{x};\mathcal{S})\rangle \to k_m, \quad \langle \mu(\mathbf{x};\mathcal{S})\rangle \to \mu_m. \tag{7.9}$$

To get the cluster bounds on the elastic moduli, consider the trial fields

$$\mathbf{u}(\mathbf{x};\mathcal{S}) = \mathbf{E}\cdot\mathbf{x} + \lambda\iint \mathbf{u}^{(1)}(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}, \tag{7.10}$$

which represent the counterpart of the fields (4.7), (4.12) in the scalar case, and apply the variational principle of the type (4.6):

$$\mathbf{E} : \mathbb{L}^* : \mathbf{E} \le W[\mathbf{u}(\cdot)] = \Big\langle \nabla\mathbf{u}^{(1)}(\mathbf{x};\mathcal{S}) : \mathbb{L}(\mathbf{x};\mathcal{S}) : \nabla\mathbf{u}^{(1)}(\mathbf{x};\mathcal{S})\Big\rangle. \tag{7.11}$$

In (7.11)

$$\mathbb{L}^* = k^*\mathbb{J}' + 2\mu^*\mathbb{J}'' \tag{7.12}$$

is the effective elastic moduli tensor of the dispersion of spheroids under study.

Inserting the trial fields (7.10) into the energy functional (7.11) makes the latter a quadratic function of λ

$$W = W(\lambda) = A - 2B\lambda + C\lambda^2, \tag{7.13}$$

with the coefficients

$$A = \mathbf{E} : \langle \mathbb{L}(\mathbf{x};\mathcal{S})\rangle : \mathbf{E}, \tag{7.14a}$$

$$B = \mathbf{E} : \mathbb{L}_m : \iiint h(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1)\,\boldsymbol{\varepsilon}^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2) \times \langle \psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2, \tag{7.14b}$$

$$\begin{aligned} C = {} & \iiint \boldsymbol{\varepsilon}^{(1)}(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1) : \mathbb{L}_m : \boldsymbol{\varepsilon}^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2)\langle \psi'(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2 \\ & - \iiint h(\mathbf{x}-\mathbf{y}_1;\boldsymbol{\omega}_1)\,\boldsymbol{\varepsilon}^{(1)}(\mathbf{x}-\mathbf{y}_2;\boldsymbol{\omega}_2) : \mathbb{L}_m : \boldsymbol{\varepsilon}^{(1)}(\mathbf{x}-\mathbf{y}_3;\boldsymbol{\omega}_3) \\ & \times \langle \psi(\mathbf{y}_1;\boldsymbol{\omega}_1)\psi'(\mathbf{y}_2;\boldsymbol{\omega}_2)\psi'(\mathbf{y}_3;\boldsymbol{\omega}_3)\rangle\,\mathrm{d}\mathbf{y}_1\mathrm{d}\mathbf{y}_2\mathrm{d}\mathbf{y}_3\,\mathrm{d}\boldsymbol{\omega}_1\mathrm{d}\boldsymbol{\omega}_2\mathrm{d}\boldsymbol{\omega}_3. \end{aligned} \tag{7.14c}$$

Optimizing (7.13) with respect to λ gives

$$\mathbf{E} : \mathbb{L}^* : \mathbf{E} \le \mathbf{E} : \mathbb{L}^{\rm cl} : \mathbf{E}, \quad \mathbf{E} : \mathbb{L}^{\rm cl} : \mathbf{E} = \lim_{w\to 0} \left(A - \frac{B^2}{C} \right), \tag{7.15}$$

thus providing obviously an upper bound, $\mathbb{L}^{\rm cl}$, on the effective elastic moduli tensor $\mathbb{L}^*$. This will be exactly the first-order cluster bound of Torquato for the microcracked elastic solid under study. Its evaluation will be briefly reported in the next Section.

8. EVALUATION OF THE CLUSTER BOUND IN THE ELASTIC CASE

First, as it follows from (7.9),

$$\lim_{w\to 0} A = \mathbf{E} : \mathbb{L}_m : \mathbf{E}. \tag{8.1}$$

Next, for the coefficient B [see (7.14b)], we have, similarly to (5.4), $B = nB_1 - n^2 B_2$, where

$$B_1 = \mathbf{E} : \mathbb{L}_m : \iint h(\mathbf{z};\boldsymbol{\omega})\, \boldsymbol{\varepsilon}^{(1)}(\mathbf{z};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, {\rm d}\mathbf{z}\, {\rm d}\boldsymbol{\omega},$$

$$B_2 = \mathbf{E} : \mathbb{L}_m : \iiiint h(\mathbf{z}_1;\boldsymbol{\omega}_1)\, \boldsymbol{\varepsilon}^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2) R(\mathbf{z}_1 - \mathbf{z}_2)\, P(\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_2)\, {\rm d}\mathbf{z}_1 {\rm d}\mathbf{z}_2\, {\rm d}\boldsymbol{\omega}_1 {\rm d}\boldsymbol{\omega}_2.$$

But, due to (7.3) and (7.6), $B_1 = V_\omega \mathbf{E} : \overline{\mathbb{B}} : \mathbf{E}$, so that

$$\lim_{w\to 0} B_1 = V_a\, \mathbf{E} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E}$$

with the tensor $\overline{\mathbb{B}}^{\,\omega}$ defined in (7.6a).

The coefficient B_2 in the "crack" limit vanishes, since it can be recast as

$$\lim_{w\to 0} B_2 = \mathbf{E} : \mathbb{L}_m : \iint {\rm def}\, \mathbf{U}^{(1)}(\mathbf{z}_2) \left[\lim_{w\to 0} \int_\Omega h(\mathbf{z}_1;\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_1)\, {\rm d}\boldsymbol{\omega}_1 \right] R(\mathbf{z}_1 - \mathbf{z}_2)\, {\rm d}\mathbf{z}_1 {\rm d}\mathbf{z}_2 = 0, \tag{8.2}$$

where

$$\mathbf{U}^{(1)}(\mathbf{x}) = \lim_{w\to 0} \int_\Omega \mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, {\rm d}\boldsymbol{\omega} \tag{8.3}$$

is a field which can be easily shown to be finite everywhere [similarly to the field $U^{(1)}(\mathbf{x})$ in Section 3, see (3.8)]; the term in the square brackets in (8.2) vanishes in the limit $w \to 0$, again due to (2.10a). Hence,

$$\lim_{w\to 0} B = n \lim_{w\to 0} B_1 = \alpha\, \mathbf{E} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E}; \tag{8.4}$$

$\alpha = \alpha_3 = nV_a$ since only the 3-D case is treated in this Section.

For the coefficient C [see (7.13c)], the same virial expansion (5.10) applies with appropriate values of the factors C_1, C_2 and C_3. Note immediately that the three-point statistics

once again does not show up [in both 2-D and 3-D], since the n^3-coefficient C_3 vanishes. The reason is that it can be recast in the "crack" limit as

$$\lim_{w\to 0} C_3 = \lim_{w\to 0}\, w \iiint H_d(|\mathbf{z}_1|/a)\, h_a(|\mathbf{z}_1|)\, \nabla\mathbf{U}^{(1)}(\mathbf{z}_2) : \mathbb{L}_m : \nabla\mathbf{U}^{(1)}(\mathbf{z}_3)$$

$$\times \Big[\, g_3(\mathbf{z}_1,\mathbf{z}_2,\mathbf{z}_3) - 1 + R(\mathbf{z}_{1,2}) + R(\mathbf{z}_{1,3})\Big]\, \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \mathrm{d}\mathbf{z}_3 = 0, \tag{8.5}$$

see (A.17), since the field $\mathbf{U}^{(1)}(\mathbf{x})$, defined in (8.3), remains finite in the same limit.

In turn, for the n-coefficient C_1 we have now

$$n \lim_{w\to 0} C_1 = \alpha\, \mathbf{E} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E}, \tag{8.6}$$

having integrated by parts and using, similarly to the scalar case, eqn (7.4) for the single inclusion field $\boldsymbol{\varepsilon}^{(1)}(\mathbf{x},\boldsymbol{\omega})$. [All fourth-rank tensors hereafter, being isotropic, commute, e.g. $\mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} = \overline{\mathbb{B}}^{\,\omega} : \mathbb{L}_m$, etc.]

Finally, for the n^2-coefficient C_2 the representations (5.10) and (A.2) can be written down once more with, for instance, $\nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\cdot\nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})$ replaced by $\nabla\mathbf{u}^{(1)}(\mathbf{z};\boldsymbol{\omega}) : \mathbb{L}_m : \nabla\mathbf{u}^{(1)}(\mathbf{z};\boldsymbol{\omega})$. Manipulations, entirely similar to the scalar case [see Appendix A], give

$$C_2 = -C_{21} = -\iint R(\mathbf{z}_1-\mathbf{z}_2)$$

$$\times \Big[\int_\Omega \nabla\mathbf{u}^{(1)}(\mathbf{z}_1;\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_1)\, \mathrm{d}\boldsymbol{\omega}_1\Big] : \mathbb{L}_m : \Big[\int_\Omega \nabla\mathbf{u}^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2) P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_2\Big]\, \mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2,$$

which, having integrating by parts twice with respect to the spatial variables and taking again (7.4) into account, yields in the "crack" limit

$$n^2 \lim_{w\to 0} C_2 = -\alpha^2\, \mathbf{E} : \overline{\mathbb{B}}^{\,\omega} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E}. \tag{8.7}$$

Equations (8.1) and (8.4) to (8.7), when inserted into (7.15), give the cluster bound

$$\mathbf{E} : \mathbb{L}^{\mathrm{cl}} : \mathbf{E} = \mathbf{E} : \mathbb{L}_m : \mathbf{E} - \frac{\alpha(\mathbf{E} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E})^2}{\mathbf{E} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E} + \alpha\mathbf{E} : \overline{\mathbb{B}}^{\,\omega} : \mathbb{L}_m : \overline{\mathbb{B}}^{\,\omega} : \mathbf{E}}\,, \tag{8.8}$$

which, due to the isotropy of all fourth-rank tensors, entering (8.8), reduces to the following estimates on the effective bulk and shear moduli of the microcracked solid under study:

$$k^* \le k^{\mathrm{cl}}\,, \quad \mu^* \le \mu^{\mathrm{cl}}, \tag{8.9}$$

where

$$\frac{k^{\mathrm{cl}}}{k_m} = \frac{1}{1+\alpha\overline{k}^{\,\omega}} = \left\{1 + \frac{4}{3\pi}\,\frac{1-\nu_m^2}{1-2\nu_m}\,\alpha\right\}^{-1}, \tag{8.9a}$$

$$\frac{\mu^{\mathrm{cl}}}{\mu_m} = \frac{1}{1+2\alpha\overline{\mu}^{\,\omega}} = \left\{1 + \frac{8}{15\pi}\,\frac{(1-\nu_m)(5-\nu_m)}{2-\nu_m}\,\alpha\right\}^{-1}. \tag{8.9b}$$

The bounds (8.9) represent the eventual form of the three-point cluster bounds of Torquato for a cracked solid [in 3-D] with randomly oriented penny-shaped cracks.

Similarly to the scalar case [Section 5], the bounds (8.9) admit a simple interpretation, coinciding with the "approximation of the non-interacting cracks." Recall that the latter corresponds to the situation when each crack is considered as isolated and immersed into the homogeneous stress field $\mathbb{L}_m^{-1} : \mathbf{E}$ that equals the stress in the virgin matrix. The effective compliance $\mathbb{L}^{*-1}$ in this case is a linear function of the crack density α which, upon averaging over cracks' orientations, brings forth the formulae (8.9) [see Kachanov, 1992]. Numerous computer simulations, reported by Kachanov (1992) and Mauge and Kachanov (1994), indicate that the aforementioned approximation remains accurate at high crack densities, provided the mutual positions of cracks are random. The explanation, proposed by the authors, is the approximate cancellation of the competing interaction effects of shielding and amplifying, due to the fact that the average [macroscopic] stress tensor is unaffected by the presence of cracks. A key question, posed by Kachanov (1992, p. 321) in this connection, is whether the interactions increase or reduce the effective moduli as compared to those for non-interacting cracks. The bounds (5.15) and (8.9) allow us to offer a rigorous answer to this question. Namely, in the statistically isotropic case and under the basic assumptions (2.2) and (2.3) of lack of correlations between location and orientation of cracks, the cracks' interactions always decrease the effective properties [conductivity and elastic moduli] of the solid.

It is also noted that the bounds (8.9) coincide with the prescriptions of the Mori-Tanaka method, proposed by Benveniste (1987) as certain approximations for the effective bulk and shear moduli of a microcracked solid. Hence it turns out that the latter prescriptions represent rigorous bounds on the effective elastic moduli of randomly microcracked solids. The formulae (8.9) however seem to have appeared for the first time in Kanaun (1980) as approximations of the effective field type for the elastic moduli of a solid, containing a Poissonian set of microcracks [see also Kanaun and Levin, 1994, for more details of the approach]. In the dilute case, i.e. to the order $O(\alpha)$, the bounds (8.9) reproduce the rigorous results of Bristow (1960) and Walsh (1965).

9. DISCUSSION

In the present paper we have introduced and developed a formalism for a rigorous treatment of microcracked solids by means of marked random point processes. The first and simplest application, chosen here for illustrating the needed technique and the typical problems that may be expected in further studies, is the evaluation of the cluster bounds of Torquato, and of certain their generalizations, for such solids. The obtained results have a simple form: the bound (5.15) and (8.9) on the effective conductivity and elastic moduli, respectively. The bounds themselves deserve a more thorough discussion since their eventual appearance here is a bit surprising and unexpected at first glance.

The first and the most important fact to be pointed out is that the two- and three-point statistics do not influence the cluster bounds for a microcracked solid. The underlying reason for this independence is not entirely clear to the author. A certain explanation may be sought in the very geometrical nature of the inhomogeneities under studies—i.e. of the

cracks—which possess infinitesimally small thickness along the cuts in the medium, and hence represent lower dimension [$(N-1)$-D] defects immersed into an N-D medium, $N = 2, 3$. This observation suggests that the statistics could explicitly enter the final expressions for the bounds only if a kind of "surface-surface" correlations, similar to those introduced by Doi (1976) in a different homogenization context, are incorporated into the trial fields from the very beginning. The detailed discussion of this possibility and of its implications lies however beyond the scope of the present study. We shall only recall that the situation when the thickness of the inclusions is finite [i.e. the dimension of the defects and of the medium coincide] is drastically different, as is well known. For example, for a dispersion of nonoverlapping spheres, when the cluster and Beran's bounds coincide, both the two-and three point spatial statistics of sphere centers considerably influence the bounds, as is well seen from the results of Felderhof (1982) and Beasley and Torquato (1986).

Second, the fact that the three-point statistics does not influence the energy for the class of trial fields under study indicates that the bounds, obtained by means of the classical and by the Hashin-Shtrikman (HS) variational principles, should coincide as a matter of fact. Recall that this follows from the elucidating derivation of the HS principle due to Hill (1963b), through neglecting sign-definite terms in the energy functional that depend on the three-point statistics. This remark explains why the HS-type bounds on the elastic moduli for microcracked solids, recently derived by Ponte Castañeda and Willis (1995), are tighter than the cluster bounds (8.9), found here by means of the "more powerful" classical principle. Indeed, in the foregoing cluster bound procedure, the trial fields (7.10) contain only one adjustable scalar parameter λ. At the same time, in the HS-procedure used by Ponte Castañeda and Willis (1995), the cracked body is considered as containing different families of ellipsoids [degenerating into cracks], each one of fixed orientation. Then the polarization field is taken step-constant, but with different values in each family, which obviously permits to command a bigger amount of adjustable parameters than in the cluster procedure. Due to the same reasons, a similar HS-procedure, when applied to the scalar conductivity problem of Section 5, will produce a bound on the effective conductivity, sharper than the cluster one (5.15).

It is to be remarked finally that the HS-procedure of Ponte Castañeda and Willis (1995) suggests a natural generalization of the cluster trial fields like (7.10). Namely, one can assume that the scalar λ there depends upon orientation $\boldsymbol{\omega}$. The fields (7.10) are then replaced by

$$\mathbf{u}(\mathbf{x};\mathcal{S}) = \mathbf{E}\cdot\mathbf{x} + \int\!\!\int \lambda(\boldsymbol{\omega})\mathbf{u}^{(1)}(\mathbf{x}-\mathbf{y};\boldsymbol{\omega})\psi'(\mathbf{y};\boldsymbol{\omega})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\boldsymbol{\omega}, \tag{9.1}$$

and the adjustable quantity is now the function $\lambda(\boldsymbol{\omega})$, defined over the "mark" space, i.e. over the unit sphere Ω [or unit circle in 2-D]. Another possible generalization is to choose $\mathbf{u}^{(1)}(\mathbf{x};\boldsymbol{\omega})$ in (7.10) or (9.1) again as the single spheroid field, but for the case of a matrix with adjustable elastic moduli k_0, μ_0. This will bring forth, besides the scalar λ [or the function $\lambda(\boldsymbol{\omega})$], a second adjustable quantity [the dimensionless ratio k_0/μ_0] in the energy functional (7.11). The detailed analysis of these possibilities is nontrivial and, once again, goes far beyond the aim of the present paper—introduction and "promotion" of the marked sets of random points as a natural tool in studying the effective behaviour of microcracked solids.

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APPENDIX A: EVALUATION OF THE COEFFICIENTS C's

The coefficients C's that enter (5.12), have the forms

$$C_{11} = \iint_{\Omega} |\, \nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\,|^2 P(\boldsymbol{\omega})\,\mathrm{d}\mathbf{z}\,\mathrm{d}\boldsymbol{\omega}, \tag{A.1a}$$

$$C_{12} = \iint_{\Omega} h(\mathbf{z};\boldsymbol{\omega})\,|\,\nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\,|^2 P(\boldsymbol{\omega})\,\mathrm{d}\mathbf{z}\,\mathrm{d}\boldsymbol{\omega}, \tag{A.1b}$$

$$C_{21} = \iint R(\mathbf{z}_1-\mathbf{z}_2)\left[\int_{\Omega}\nabla T^{(1)}(\mathbf{z}_1;\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_1)\,\mathrm{d}\boldsymbol{\omega}_1\right]\cdot\left[\int_{\Omega}\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)P(\boldsymbol{\omega}_2)\,\mathrm{d}\boldsymbol{\omega}_2\right]\,\mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2, \tag{A.2a}$$

$$C'_{22} = \iint R(\mathbf{z}_1-\mathbf{z}_2)\left[\int_{\Omega}h(\mathbf{z}_1;\boldsymbol{\omega}_1)\nabla T^{(1)}(\mathbf{z}_1;\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_1)\,\mathrm{d}\boldsymbol{\omega}_1\right] \cdot\left[\int_{\Omega}\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)P(\boldsymbol{\omega}_2)\,\mathrm{d}\boldsymbol{\omega}_2\right]\,\mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2, \tag{A.2b}$$

$$C''_{22} = \iint R(\mathbf{z}_1-\mathbf{z}_2)\left[\int h(\mathbf{z}_1;\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_1)\,\mathrm{d}\boldsymbol{\omega}_1\right]\left[\int |\,\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\,|^2\,P(\boldsymbol{\omega}_2)\,\mathrm{d}\boldsymbol{\omega}_2\right]\,\mathrm{d}\mathbf{z}_1\mathrm{d}\mathbf{z}_2, \tag{A.2c}$$

$$C_{23} = \iint h(\mathbf{z}_1;\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_1)\,\mathrm{d}\boldsymbol{\omega}_1\,\mathrm{d}\mathbf{z}_1\left[\int |\,\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\,|^2\,P(\boldsymbol{\omega}_2)\,\mathrm{d}\boldsymbol{\omega}_2\,\mathrm{d}\mathbf{z}_2\right], \tag{A.2d}$$

$$C_3 = \iiiint\!\!\iint h(\mathbf{z}_1;\boldsymbol{\omega}_1)\,\nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\cdot\nabla T^{(1)}(\mathbf{z}_3;\boldsymbol{\omega}_3) \times G_3(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)P(\boldsymbol{\omega}_1)P(\boldsymbol{\omega}_2)P(\boldsymbol{\omega}_3)\,\mathrm{d}\mathbf{z}_1\,\mathrm{d}\mathbf{z}_2\,\mathrm{d}\mathbf{z}_3\,\mathrm{d}\boldsymbol{\omega}_1\,\mathrm{d}\boldsymbol{\omega}_2\,\mathrm{d}\boldsymbol{\omega}_3. \tag{A.2e}$$

To evaluate C_{11}, integrate by parts in (A.1a) and use (3.1) for the single spheroid field $T^{(1)}(\mathbf{z};\boldsymbol{\omega})$. This yields

$$C_{11} = V_{\omega}\mathbf{G}\cdot\int_{\Omega}[\,\mathbf{I}+\mathbf{B}(\boldsymbol{\omega})\,]\cdot\mathbf{B}(\boldsymbol{\omega})\,P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega}\cdot\mathbf{G}. \tag{A.3}$$

As far as the coefficient C_{12} is concerned [see (A.1b)], employ (4.2)

$$C_{12} = V_{\omega}\mathbf{G}\cdot\int_{\Omega}\mathbf{B}(\boldsymbol{\omega})\cdot\mathbf{B}(\boldsymbol{\omega})\,P(\boldsymbol{\omega})\,\mathrm{d}\boldsymbol{\omega}\cdot\mathbf{G},$$

which means that

$$C_1 = C_{11}-C_{12} = B_1 \quad\text{and thus}\quad \lim_{w\to 0}C_1 = \lim_{w\to 0}B_1 \tag{A.4}$$

[see (5.6)]. The value of

$$\lim_{w\to 0} B_1,$$

let us recall, is given in both 2-D and 3-D cases in (5.7).

Before evaluating

$$\lim_{w\to 0} C_{21},$$

we shall first show that

$$\lim_{w\to 0} C'_{22} = \lim_{w\to 0} C_{21}. \tag{A.5}$$

Indeed, recast C'_{22} [see (A.2b)] as

$$C'_{22} = \iint R(\mathbf{z}_1 - \mathbf{z}_2) \left[\int_\Omega h(\mathbf{z}_1;\boldsymbol{\omega}_1) \left[\mathbf{G} + \nabla T^{(1)}(\mathbf{z}_1;\boldsymbol{\omega}_1) \right] P(\boldsymbol{\omega}_1)\, \mathrm{d}\boldsymbol{\omega}_1 \right]$$

$$\cdot \left[\int_\Omega \nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2) P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_2 \right] \mathrm{d}\mathbf{z}_1 \mathrm{d}\mathbf{z}_2,$$

since the term, contributed through adding $\mathbf{G}$, is proportional to the volume V_ω [or surface S_ω in 2-D] of the ellipsoid [ellipse] and therefore it vanishes in the limit $w \to 0$. Integrating appropriately by parts and using (3.1) for the field $T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)$ at $\kappa_f = 0$, easily yields (A.5).

To evaluate

$$\lim_{w\to 0} C_{21},$$

recast it as

$$\lim_{w\to 0} C_{21} = \lim_{w\to 0} \iint P(\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_1 \mathrm{d}\boldsymbol{\omega}_2 \iint R(\mathbf{z}_1 - \mathbf{z}_2)\, \nabla T^{(1)}(\mathbf{z}_1;\boldsymbol{\omega}_1) \cdot \nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\, \mathrm{d}\mathbf{z}_1 \mathrm{d}\mathbf{z}_2.$$

An appropriate integration by parts with respect to the spatial coordinates, combined with application of (3.1) [at $\kappa_f = 0$], gives

$$\lim_{w\to 0} C_{21} = \lim_{w\to 0} \iint P(\boldsymbol{\omega}_1) P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_1 \mathrm{d}\boldsymbol{\omega}_2 \iint h(\mathbf{z}_1;\boldsymbol{\omega}_1) h(\mathbf{z}_2;\boldsymbol{\omega}_2) R(\mathbf{z}_1 - \mathbf{z}_2)$$

$$\times\, \mathbf{G} \cdot [\mathbf{I} + \mathbf{B}(\boldsymbol{\omega}_1)] \cdot [\mathbf{I} + \mathbf{B}(\boldsymbol{\omega}_2)]\, \mathrm{d}\mathbf{z}_1 \mathrm{d}\mathbf{z}_2 \cdot \mathbf{G}$$

$$= K_d^2 \mathbf{G} \cdot \iint \mathbf{e}_{\boldsymbol{\omega}_1} \mathbf{e}_{\boldsymbol{\omega}_1} P(\boldsymbol{\omega}_1)\, \mathrm{d}\boldsymbol{\omega}_1 \cdot \iint \mathbf{e}_{\boldsymbol{\omega}_2} \mathbf{e}_{\boldsymbol{\omega}_2} P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_2 \cdot \mathbf{G} = \frac{K_d^2}{d^2} V_a^2 G^2, \tag{A.6}$$

since $R(\mathbf{z}_1 - \mathbf{z}_2) = 1$ [because $|\mathbf{z}_1|, |\mathbf{z}_2| \le a$ imply $|\mathbf{z}_1 - \mathbf{z}_2| < 2a$ and hence $g(|\mathbf{z}_1 - \mathbf{z}_2|) = 0$ due to the assumption of nonoverlapping].

The key point is the evaluation in the "crack" limit of the coefficient C''_{22}, defined in (A.2c), i.e. the quantity

$$\lim_{w\to 0} C''_{22}.$$

The reason is that this is the only term through which the two-point statistics of the cracks' spatial distribution may enter the bound κ^{cl}.

To calculate

$$\lim_{w\to 0} C''_{22}$$

insert into the integral (A.2c) $R(\mathbf{x}) = 1 - g(\mathbf{x})$ [see (5.3)]. Then C''_{22} splits into two parts

$$C''_{22} = \mathcal{N} - \mathcal{M}[g]. \tag{A.7}$$

Moreover,

$$\lim_{w\to 0} \mathcal{N} = \int \left[\lim_{w\to 0} \frac{1}{w} \int_\Omega h(\mathbf{z}_1;\boldsymbol{\omega}_1)\, P(\boldsymbol{\omega}_1)\, \mathrm{d}\boldsymbol{\omega}_1 \right] \mathrm{d}\mathbf{z}_1$$

$$\times \left[\lim_{w\to 0} w \int\!\!\int_\Omega |\, \nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\,|^2\, P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_2 \right] \mathrm{d}\mathbf{z}_2 = V_a \lim_{w\to 0} wC_{11},$$

having used the formula (A.1a) for C_{11}, equation (3.1) and the property (3.2) of the function $H_d(\rho)$. In turn, the expression (A.3) for C_{11} and the asymptotic (4.8) produce after obvious manipulations

$$\lim_{w\to 0} \mathcal{N} = \frac{K_d^2}{d}\, V_a^2 G^2. \tag{A.8}$$

Consider the second term in (A.7), $\mathcal{M}[g]$, which is the *only* one that depends on the two-point statistics [something reflected in its notation, underlying in this way that $\mathcal{M}[g]$ is a linear functional of the radial distribution function $g(r)$]. In the "crack" limit $w \to 0$ it has the form

$$\lim_{w\to 0} \mathcal{M}[g] = \int\!\!\int g(\mathbf{z}_1 - \mathbf{z}_2) \left[\lim_{w\to 0} \frac{1}{w} \int_\Omega h(\mathbf{z}_1;\boldsymbol{\omega}_1)\, P(\boldsymbol{\omega}_1)\, \mathrm{d}\boldsymbol{\omega}_1 \right]$$

$$\times \left[\lim_{w\to 0} w \int_\Omega |\, \nabla T^{(1)}(\mathbf{z}_2;\boldsymbol{\omega}_2)\,|^2\, P(\boldsymbol{\omega}_2)\, \mathrm{d}\boldsymbol{\omega}_2 \right] \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2$$

$$= \int\!\!\int g(\mathbf{z}_1 - \mathbf{z}_2) H_d(|\mathbf{z}_1|/a)\, h_a(\mathbf{z}_1)\, \mathcal{T}(\mathbf{z}_2)\, \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2$$

and hence

$$\lim_{w\to 0} \mathcal{M}[g] = \int \Lambda(\mathbf{z})\, \mathcal{T}(\mathbf{z})\, \mathrm{d}\mathbf{z}, \tag{A.9}$$

where

$$\mathcal{T}(\mathbf{z}) = \lim_{w\to 0} w \int_\Omega |\, \nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\,|^2\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega}, \tag{A.10}$$

$$\Lambda(\mathbf{z}) = \int g(\mathbf{z} - \mathbf{y}) H_d(|\mathbf{y}|/a)\, h_a(\mathbf{y})\, \mathrm{d}\mathbf{y}. \tag{A.11}$$

Note that in the integral (A.9) the integration is over the region $|\mathbf{z}| > a$ due to the presence of $h_a(\mathbf{y})$ in the integrand of $\Lambda(\mathbf{z})$ [see (A.11)] and the assumption of nonoverlapping ($g(\mathbf{z} - \mathbf{y}) = 0$, if $|\mathbf{z} - \mathbf{y}| < 2a$). But we shall prove in a moment that

$$\mathcal{T}(\mathbf{x}) = \frac{K_d^2}{d-1}\, \mathbf{G}\cdot(r\nabla\nabla\, r)\cdot\mathbf{G} H_d(\rho)\, h_a(\mathbf{x}), \tag{A.12}$$

$r = |\mathbf{x}|$, which implies that $\mathcal{T}(\mathbf{x}) = 0$ at $|\mathbf{x}| > a$. Hence $\mathcal{M}[g] \equiv 0$, which means that

$$\lim_{w\to 0} C''_{22} = \frac{K_d^2}{d}\, V_a^2 G^2 \tag{A.13}$$

[see (A.7) and (A.8)].

To prove (A.12), note that obviously

$$w \int_\Omega h(\mathbf{z};\boldsymbol{\omega})\, |\, \nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\, |^2\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} \le w \int_\Omega |\, \nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\, |^2\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega},$$

and take the limit $w \to 0$ in this inequality

$$0 \le \widetilde{\mathcal{T}}(\mathbf{z}) \le \mathcal{T}(\mathbf{z}), \tag{A.14}$$

where

$$\widetilde{\mathcal{T}}(\mathbf{z}) = \lim_{w\to 0}\, w \int_\Omega h(\mathbf{z};\boldsymbol{\omega})\, |\, \nabla T^{(1)}(\mathbf{z};\boldsymbol{\omega})\, |^2\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega}.$$

The field $\widetilde{\mathcal{T}}(\mathbf{z})$ can be easily evaluated, however, making use of (3.2) and (3.3):

$$\widetilde{\mathcal{T}}(\mathbf{z}) = K_d^2 \lim_{w\to 0}\, \frac{1}{w}\, \mathbf{G} \cdot \int_\Omega \mathbf{e}_\omega \mathbf{e}_\omega\, h(\mathbf{x};\boldsymbol{\omega})\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} \cdot \mathbf{G}$$

$$= \frac{K_d^2}{d-1}\, \mathbf{G} \cdot (r\nabla\nabla\, r) \cdot \mathbf{G}\, H_d(\rho)\, h_a(\mathbf{x}). \tag{A.15}$$

Due to the inequality (A.14), to prove (A.12) it suffices to show that $\int \mathcal{T}(\mathbf{z})\, \mathrm{d}\mathbf{z} = \int \widetilde{\mathcal{T}}(\mathbf{z})\, \mathrm{d}\mathbf{z}$. But

$$\int \mathcal{T}(\mathbf{z})\, \mathrm{d}\mathbf{z} = \lim_{w\to 0} wC_{11} = \lim_{w\to 0} wV_\omega\, \mathbf{G} \cdot \int \mathbf{B}(\boldsymbol{\omega}) \cdot \mathbf{B}(\boldsymbol{\omega})\, P(\boldsymbol{\omega})\, \mathrm{d}\boldsymbol{\omega} \cdot \mathbf{G} = \frac{K_d^2}{d}\, V_a G^2$$

[see (A.3)]. On the other hand, the same value of the integral $\int \widetilde{\mathcal{T}}(\mathbf{z})\, \mathrm{d}\mathbf{z}$ can be easily deduced from (A.15), if (3.3) is taken into account together with obvious symmetry arguments. Hence (A.12) indeed holds true.

Next, in virtue of (A.2d) and (A.3), one has $C_{23} = \mathcal{N}$ so that, due to (A.8),

$$\lim_{w\to 0} C_{23} = \frac{K_d^2}{d}\, V_a^2 G^2. \tag{A.16}$$

Consider finally the coefficient C_3 [see (A.2e)], through which the three-point statistics of the crack centers may only enter the bound (4.14). But it is easily seen that it also vanishes in the "crack" limit since it can be recast as

$$\lim_{w\to 0} C_3 = \lim_{w\to 0}\, w \iiint H_d(|\mathbf{z}_1|/a)\, h_a(\mathbf{z}_1)$$

$$\times\, \nabla U^{(1)}(\mathbf{z}_2) \cdot \nabla U^{(1)}(\mathbf{z}_3) G_3(\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3)\, \mathrm{d}\mathbf{z}_1\, \mathrm{d}\mathbf{z}_2\, \mathrm{d}\mathbf{z}_3 = 0, \tag{A.17}$$

with G_3 given in (5.10), and the field $U^{(1)}(\mathbf{x})$, defined in (3.8), which remains finite in the said limit.

Combining equations (4.4), (5.1), (5.4), (5.7), (5.11), (5.12), (A.4), (A.6), (A.13), (A.16) and (A.17) gives eventually (5.13) and hence the formula (5.15) for the cluster bound.

APPENDIX B: THE MODIFIED BERAN BOUND IN THE DILUTE CASE

With the same notations (5.4)

$$B_1 = \mathbf{G} \cdot \iint h(\mathbf{z};\boldsymbol{\omega})\, \nabla T^{(\mathrm{b})}(\mathbf{z};\boldsymbol{\omega}) P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{z}\, \mathrm{d}\boldsymbol{\omega}$$

$$= -\frac{1}{w}\, \mathbf{G} \cdot \iint h(\mathbf{z};\boldsymbol{\omega})\, \nabla\nabla\, \varphi_\omega(\mathbf{z}) P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{z}\, \mathrm{d}\boldsymbol{\omega} \cdot \mathbf{G},$$

since $T^{(\mathrm{b})}(\mathbf{z};\boldsymbol{\omega}) = -\mathbf{G} \cdot \nabla\varphi_\omega(\mathbf{z})/w$, see (4.10) and (5.5a). Using the formula (3.5) for $\nabla\nabla\, \varphi_\omega(\mathbf{z})$ within the spheroid S_ω together with obvious symmetry arguments gives

$$\lim_{w\to 0} B_1 = \frac{1}{d}\, G^2 \lim_{w\to 0} \frac{1}{w}\, V_\omega = \frac{1}{d}\, V_a G^2. \tag{B.1}$$

In turn, the needed n-coefficient of C in the case under study reads

$$C_1 = C_{11} - C_{12} = \iint_\Omega |\, \nabla T^{(\mathrm{b})}(\mathbf{z};\boldsymbol{\omega})\, |^2\, P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{z}\, \mathrm{d}\boldsymbol{\omega}$$

$$- \iint_\Omega h(\mathbf{z};\boldsymbol{\omega})\, |\, \nabla T^{(\mathrm{b})}(\mathbf{z};\boldsymbol{\omega})\, |^2\, P(\boldsymbol{\omega})\, \mathrm{d}\mathbf{z}\, \mathrm{d}\boldsymbol{\omega}, \tag{B.2}$$

see (5.12) and (A.1a,b). Integrating by parts in the first integral in (B.2) and using once again the formula (3.5) for $\nabla\nabla\, \varphi_\omega(\mathbf{z})$ within the spheroid S_ω yields, after simple manipulations,

$$\lim_{w\to 0} C_1 = \frac{1}{d}\, G^2 \lim_{w\to 0} \frac{1}{w^2} \left[1 - \left(1 - \frac{1}{K_d}\, w\right)^2\right] V_\omega = \frac{2}{dK_d}\, V_a G^2. \tag{B.3}$$

Hence, upon combining (B.1) and (B.3),

$$\frac{\kappa^b}{\kappa_m} = 1 - n \lim_{w\to 0} \frac{B_1^2}{C_1} + o(n) = 1 - \frac{K_d}{2d}\, \alpha_d + o(\alpha_d),$$

so that the term, linear in crack density α_d, of the modified Beran bound, κ^b, is *twice* smaller than the exact value $-K_d/d$.