
Elementary Micromechanics of Heterogeneous Media

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ABSTRACT. The introductory and more elementary ideas and results of micromechanics of heterogeneous media are collected in the survey. The central problem under discussion is “homogenization.” It replaces such media by homogeneous ones, which behave macroscopically in the same way and possess certain gross effective properties. These properties are related in a complicated manner to the prescribed internal structure of the medium and their evaluation, in general, represents a profound challenge in any specific situation. A brief historical survey is given, underlying the reappearance of essentially the same “homogenization” quest in numerous guises and contexts over the last two centuries. Within the framework of the volume-averaging approach the basic notions are introduced and some of the central, now classical, results are then derived and discussed such as perturbation expansions, Hashin-Shtrikman’s bounds, variational estimates and Levin’s cross-property relation. A general “one-

particle” scheme for approximate evaluation of the effective properties (in the static case) is detailed in its various implementations like self-consistency, iterated limits and effective field. Illustrations concern conductivity, elasticity, and absorption phenomena in heterogeneous particulate media, as well as a simple self-consistent model for polycrystals’ homogenization.

1.1 Introduction

1.1.1 The Aim of Micromechanics

Continuum mechanics deals with ideal homogeneous materials. Its aim is to describe their response to external exertions using appropriate constitutive relations. The latter generally are specified by means of macroscopical experiments without microstructural considerations. It is a trivial statement, however, that any sample of material is microscopically inhomogeneous, even if it appears homogeneous at some natural scale of observation. Inevitably, therefore, a description of any material in terms of continuum mechanics is an approximation, and any experimental determination of constitutive behavior yields, in fact, a relationship between the “overall” properties measured in the experiment. This observation leads us to a fundamental and widespread problem of science and technology, concerning “micro-macro” interconnection, i.e. a proper and reliable determination of the macroscopic (or “large” scale) behavior of a medium which exhibits microscopic (or “small” scale) heterogeneity, on the base of the appropriate and available microstructural information. (The exact meaning of “large” and “small” depends on the specific problems and media under study.) The oldest problem of such a type, fundamental in statistical physics, is description of matter in terms of its molecular constituents. Here “small” corresponds obviously to molecular dimensions.

Micromechanics, in general, deals with heterogeneous media for which “small” has a certain intermediate dimension ℓ which is large compared to molecular dimensions, but is small in macroscale. The length ℓ is connected with the characteristic size of the heterogeneities in the medium, say, with mean radius of inclusions, voids, fibers, the

size of a crystallite in polycrystalline aggregates, etc. Though the molecular effects are not present, as a rule, in such a scale, many of the methods used in the appropriate theories have their direct origin in statistical physics and statistical mechanics, as we shall point out below. The aim of micromechanics is just to relate the gross macroscopical behavior of heterogeneous media, characterized with the above mentioned length scale ℓ , to the details of their microscopical constitution. The basic idea is that of *homogenization*, which consists in a replacement of a piece of a microheterogeneous solid by a homogeneous one which, from a macroscopical point of view “behaves” in the same manner as this piece. This fundamental idea will be briefly illustrated in the next subsection, before considering it more rigorously and in needed detail in Section 1.2.

Note that an important class of heterogeneous media, extensively treated by micromechanics, are the composites—man-made mixtures mixtures of two or more constituents, firmly (as a rule, but not always) bonded together. Among other reasons, technological demands have stimulated a very extensive bulk of studies, devoted to their gross mechanical behavior, like elasticity, strength, etc., as predefined by a specific microstructural arrangement. A considerable part of the more fundamental works along this line will be discussed in what follows. There are, however, plenty of micromechanical problems not directly concerned with mechanical properties, but representing particular cases of the same “micro-macro” interconnection quest, in which the same idea of homogenization applies.¹ An example is furnished by the problem of describing propagation of electromagnetic or acoustic waves through a heterogeneous solid or a turbulent fluid. Another example is cooling of a heated body by means of a system of tubes or holes, kept at a fixed temperature. Mathematically the latter problem is very closely connected to describing the gross behavior of a diffusing species in a medium, containing absorbing sinks. The

¹It is more precise perhaps to speak about “micro-physical” problems, instead of micromechanical since, say, diffusion, electromagnetic waves, etc., have little to do with mechanics in its classical sense. However, introducing the term physics would inevitably enlarge this survey far beyond the admissible length and (more important)—the author’s competence. In this connection it seems appropriate to recall the Constitution of the International Society for the Interaction of Mechanics and Mathematics (ISIMM), where one reads that “*Mechanics is understood here in the broad sense of the word, including relevant physical phenomena such as electromagnetic and thermal fields.*”

third example to be specially mentioned concerns the viscous flow through a porous solid (which itself could deform due to the flow).

1.1.2 The Idea of Homogenization

To illustrate the basic ideas of homogenization as simply as possible, consider a (linear) elastic heterogeneous medium. Let, for example, the tensile stress-strain behavior of the medium along the axis x_1 be under investigation. Imagine to this end that a large, say, cubical specimen \mathcal{V} with a side L is cut out from the medium; large means here that $L \gg \ell$, where ℓ is the above mentioned microscale length. Either the cube would be loaded to some level and its extension measured, or else it would be extended by some amount and the load measured. Then the stress component σ_{11} would be taken as load divided by area of the cross-section L^2 and the strain component ε_{11} as extension divided by the original length L . These two ways to find ε_{11} and σ_{11} are obvious, if the cube were homogeneous; the heterogeneity results, however, in non-homogeneous and rapidly oscillating in the microscale fields of both stress and strain. The latter quantities, calculated from the experiment, thus represent, in fact, averages of the actual forces and displacements in the cube. More precisely, they are just the so-called volume (or spatial) averages, to be denoted by overbar:

$$\bar{\varepsilon}_{11} = \frac{1}{V} \int_{\mathcal{V}} \varepsilon_{11}(\mathbf{x}) \, d\mathbf{x}, \quad \bar{\sigma}_{11} = \frac{1}{V} \int_{\mathcal{V}} \sigma_{11}(\mathbf{x}) \, d\mathbf{x}; \quad (1.1)$$

hereafter $V = \text{vol } \mathcal{V}$ is the volume of the region \mathcal{V} .

In turn, the proportionality coefficient

$$E_{11}^{\mathcal{V}} = \bar{\sigma}_{11} / \bar{\varepsilon}_{11} \quad (1.2)$$

defines the effective (or gross) Young modulus for the specimen (along the axis x_1). This means that the cube, through the relation (1.2), is “homogenized” in the sense that its heterogeneity is smoothed out and it is replaced by a homogeneous one, possessing the gross Young modulus $E_{11}^{\mathcal{V}}$.

If we now repeat the same procedure for other cubical samples of the material, of the same size and orientation as the first, we shall in general obtain slightly different values of $E_{11}^{\mathcal{V}}$, since the interior phase geometry will not be the same in full detail. This explains why the superscript ‘ \mathcal{V} ’ explicitly appeared in the notation $E_{11}^{\mathcal{V}}$.

To define a “true” material property from such experiments, i.e. one that is connected with the heterogeneous medium and its internal structure, independently of the specific choice of the subvolumes, two natural procedures can be employed.

First, perform a great number, N , of experiments on differently centered cubes (otherwise identical and identically oriented), and measure the appropriate values $E_{11}^{\mathcal{V}'}$, $E_{11}^{\mathcal{V}''}$, etc., for each one. Then, to suppress the specimen’s dependence, it is natural to define

$$E_{11}^* = \frac{1}{N} \left(E_{11}^{\mathcal{V}'} + E_{11}^{\mathcal{V}''} + \dots \right), \quad (1.3)$$

which is already a true material property. The right-hand side of (1.3) is the simplest example of the so-called *ensemble averaging*. The meaning is that to obtain information about the expected gross behavior of a heterogeneous medium, we should deal with average reaction of a whole *ensemble* of specimens of identical shape and size, and apply identical external influence. (In the foregoing reasoning these are simply the cubes taken from different parts of a big piece of the medium.) The ensemble averaging is one of the basic notion in the theory of heterogeneous media of random constitution, see e.g. the book of Beran [BEi]. An elucidating introduction, together with basic methods and ideas concerning homogenization for such random media, can be found as well in the lectures of Willis [Wle].

We shall be concerned in the present survey, however, with more elementary aspects of the theory, without invoking the proper mathematical framework for random internal constitution. That is why only the volume averaging (1.1) will be used throughout. It appears in a natural way, if a *second kind* of mental experiment is performed. Take a cube with a fixed center and start increasing its side L (assuming the medium unbounded). Then it is equally natural to expect that in the limit $L/\ell \rightarrow \infty$ the sample dependence will disappear:

$$E_{11}^{\mathcal{V}} = E_{11}^*(1 + \mathcal{O}(\ell/L)) \quad \text{as} \quad \ell/L \rightarrow 0, \quad (1.4)$$

where the *same* effective modulus E_{11}^* , as in (1.3), shows up. Hence, we shall be on the safe side, equating E_{11}^* with $E_{11}^{\mathcal{V}}$, provided the volume \mathcal{V} is big enough compared to the typical inhomogeneity, i.e. if $L \gg \ell$. But this was a basic assumption, already adopted for the class of heterogeneous media under study at the beginning of this

subsection. The importance of this assumption will be once more emphasized in Section 1.2.1, when formulating Hashin's MMM principle.

Hereafter we shall consider only media for which the ensemble and volume averages coincide; they are called *ergodic*.

A satisfactory proof of the statement that a medium is ergodic, i.e. the two definitions (1.3) and (1.4) yield, in particular, one and the same value of E_{11}^* is not a trivial matter. Such a statement amounts to the so-called *ergodic hypothesis*. It can be rigorously justified under certain additional conditions imposed on the microgeometry of the media, the most important of which is the macroscopic (or statistical) homogeneity, see again the book [BEi] for a brief, but elucidating discussion.

Intuitively, the coincidence between the ensemble and volume averages should not be a surprise, since E_{11}^* is to be specified by the medium's microgeometry solely. Any natural definition of the homogenization properties, in which sample dependence is somehow eliminated, should then result in a true and *unique* material characteristics.

Fully similar considerations can be repeated almost literally, using different physical backgrounds, chosen and tailored by the personal taste of the reader. For example, instead of elasticity, diffusion of a solute through the same cube \mathcal{V} can be considered, fixing the solute concentration at a pair of opposite faces and, in the steady state, measuring the total amount of the solute, passing through them, see [HUa]. The dielectric context is also used very often, starting with the classical works of Mossotti [MOc], [MOd], and Faraday [FAa]; the posing of the homogenization problem in this case is very clearly explained and discussed, e.g. by Bergman [BEk]. A fully equivalent, from a mathematical point of view, context concerns heat propagation which will be mainly used in what follows. That is why we should recall here the well-known equations

$$\nabla \cdot \mathbf{q}(\mathbf{x}) = 0, \quad \mathbf{q}(\mathbf{x}) = \kappa(\mathbf{x})\nabla\theta(\mathbf{x}), \quad (1.5)$$

that govern the temperature field $\theta(\mathbf{x})$ in a medium at the absence of body sources. In Eq. (1.5) $\mathbf{q}(\mathbf{x})$ is the flux vector, and $\kappa(\mathbf{x})$ represents, for the heterogeneous body under study, a rapidly fluctuating conductivity coefficient, taking different values when the point \mathbf{x} scans

the medium. In the case of a two-phase (binary) material, which very often appear in various applications,

$$\kappa(\mathbf{x}) = \begin{cases} \kappa_1, & \text{if } \mathbf{x} \in \text{constituent '1'}, \\ \kappa_2, & \text{if } \mathbf{x} \in \text{constituent '2'}. \end{cases} \quad (1.6)$$

It should be emphasized that all the results, obtained below in the heat conduction context, are equally well applicable in the contexts of electrical conductivity, dielectric behavior and magnetic permeability. A list of analogous quantities are conveniently summarized in a table by Hashin [HAi, p. 496]. The reason is the obvious mathematical similarity between between these problems: in all of them a solenoidal vector field (say, the dielectric polarizability, or the heat flux, etc.) is “proportional” to a potential vector field (the electric field, the temperature gradient, etc.) with a proportionality coefficient (which may be a tensor) rapidly varying throughout the medium.

The second context to be more extensively used in the present paper is the already employed, for illustrative purposes, (linear) elasticity problem (see Section 1.2.7 below). The basic ideas and conclusions are the same in both cases, but their implementation in the heat conductivity case is, however, simpler, since the basic quantities—the heat flux and temperature gradient—are vectors. In the elasticity case the respective quantities are tensors (the stress and strain ones) which makes the calculations more cumbersome technically. That is why we shall concentrate in what follows primarily on the scalar conductivity problem; afterward, the elasticity counterparts of the results will be discussed more concisely.

1.1.3 Brief Historical Remarks

The homogenization quest, due to its utmost importance, has kept reappearing in various guises and contexts in the last two centuries, attracting the interest and the efforts of some of the most illustrious names in science. Here we shall try to collect some historical details, without any attempt or claim to be full and exhaustive.² One of our aims is to underline the common “micromechanical” origin

²We do not mention even the famous Darcy’s book [DAa] that initiated tremendous research on flow in porous media, and on Darcy’s law, in particular. A great number of recent developments in this field can be found in other papers of the present volume.

and nature of the appropriate problems, despite the widely different scientific communities and contexts in which they have shown up.

1.1.3.1 Navier and Cauchy

It should be recalled above all that the origin and the base of the modern continuum mechanics, as laid down by Navier and Cauchy, is to a great extent “micromechanical.” The starting point of these authors was the Newtonian picture of matter as an assemblage of “material molecules” interacting by means of central forces. In a language, used today, this is nothing but a “discrete” model and their main and great contribution in this field is the “homogenization” of such a model. More precisely, imaging the “molecules” as material points and the interaction forces depending upon their displacement from the equilibrium position, first Navier and then, almost in the same time and in a more general form, now classical, Cauchy derived³ the equations describing an elastic continuum, “spread over” the discrete model—in the sense that it macroscopically behaves *in the same way* as its underlying “molecular skeleton.” This discrete model was then put aside for more than a century and the attention, in continuum mechanics at least, was focused on the appropriate partial differential equations that formed, together with the equations of hydrodynamics, the core of research in the Mathematical Physics of the previous century.

In a new guise and on a new level, similar “homogenization” problems reappeared in continuum mechanics almost a century later when Einstein [Ela] in 1905 and Bruggeman [BRg] in 1937 considered hosts of inclusions in a fluid and in an elastic medium, respectively. In both cases the problems were again micromechanical, in the sense that homogeneous continua, spread over discrete arrays of inclusions, should be constructed. The interpretation of “micro” was of course different from the pioneering works of Navier and Cauchy, but the sense of the “homogenization” quest was the same. However, the nature of interaction between the inclusions exhibited a key new feature:

³According to Love [LOd] (see the historical survey in his introduction), the Navier *Mémoire* was presented at the French Academy in May 1821, but was published only in 1827 [NAa]. The Cauchy *Mémoire* was presented at the French Academy in September 1821, but also appeared in 1827 and 1928 in his *Exercices de mathématique*. The Cauchy derivation revisited can be found in Appendix B of the same Love book [LOd].

its magnitude already was not prescribed, like a simple elastic one, say, but instead resulted from the local disturbances of the fields like displacement, velocity, etc., generated by each single particle in the medium.

1.1.3.2 Poisson and Mossotti

With elastic bodies “homogenized,” the micromechanical studies of heterogeneous media for almost a century turned toward the gross behavior of charged materials.⁴

In 1824 Poisson presented his first *Mémoire* on the theory of magnetism at a meeting of the French Academy [POa]. There he put the basis of the theory of induced magnetism, assuming a model of a nonconducting material (we would call it a matrix today) in which small conducting particles are distributed. For magnetically isotropic bodies Poisson took the particles spherical, isotropically arranged as well, and noted that an adequate theory of magnetism can be constructed if one requires that each sphere is lying in a certain constant external field. In his second *Mémoire* [POb], he treated anisotropic magnetic solids as well, representing them as an array of thin aligned three-axial conducting ellipsoids in a matrix. In these two Poisson’s papers one can see not only the origin but the rudiments of the basic models and ideas that prevailed in the theory of heterogeneous media for almost a century after their appearance, and are still useful and applicable. In particular, the model of the so-called dispersion of nonoverlapping spheres and ellipsoids seems to have emerged for the first time in this particular (magnetic) context; the model, in general, turned out very appropriate for many heterogeneous media of particulate type (matrix-inclusion composites, say), and also in the liquid-state theory.

It was Faraday in 1838 [FAa], who employed Poisson’s ideas to dielectrics, proposing to treat them as an array of metallic spheres, immersed into an insulating material (matrix) [FAa]. But a more detailed analysis of this model was due to Mossotti [MOc] who specified the embedded particles as “material molecules,” modelled them as little conducting spheres, and described the polarization of a single one. The main contribution of Mossotti was however a method

⁴In the “electric” story we shall utilize a number of historical details, given by Wiener [WIa], Brown [BRe], Landauer [LAc] and Trimarco [TRa].

of interconnecting the micro- and macroproperties of the dispersion which turned out to be the first of the so-called “cavity” approaches, and this was the heart of his second paper [MOd]. The basic, and extremely fruitful, idea of Mossotti was to remove a material region \mathcal{C} around a point in order to evaluate the (electric) force exerted on the point, due to the interactions with the molecules outside \mathcal{C} . In this way the first of the “cavity” methods in theory of heterogeneous media emerged. The field acting on the cavity is the *local* (or effective, or internal) field that *differs* from the applied macroscopic one, as a consequence of the presence of the other molecules. In Section 1.5.3 below, when discussing the so-called effective field approach for evaluating the effective properties, we shall specially outline its connection with the “cavity” idea, see Section 1.5.5.2. As pointed out by Landauer [LAc], the Mossotti work [MOd] is based, however, on etherial concepts and notions, typical for the epoch, which makes this classical paper difficult for a modern reader to follow. The idea of local field was reintroduced and exploited by H. Lorentz around 1880. A very clear and now classical exposition of this idea and its application to dielectric and optical properties⁵ is given in his well-known book [LOb, Section 117 and App. 54].

Almost at the same time Clausius in his book [CLa, pp. 67–77] revisited Mossotti’s internal field approach in a concise way, much easier for a modern reader to follow [LAc]. He cut each molecule out of the medium and replaced the rest with a material possessing the effective dielectric constant, reaching the *explicit* and now classical formula for the latter, given in Eq. (1.19) below. This is, as a matter of fact, the first appearance of the so-called effective medium idea that much later was successfully exploited by Bruggeman, Skrohod, Hill, Budiansky *et al.* in the theory of heterogeneous solids, see Section 1.5.2 below. As pointed out by Brown [BRe], Mossotti’s paper does not contain explicitly the formula for the effective dielectric constant; Clausius’ book does, and that is why H. Lorentz [LOb, Section 124] attributes the formula (1.19) to Clausius and Mossotti,

⁵Recall that according to Maxwell, $\mu^2 = \kappa$, where κ is the dielectric constant of a transparent medium and $\mu = c/v$ is its refractivity index (i.e. the ratio c/v between the velocity of the light in the vacuum and in the medium). This classical formula of the electromagnetic theory explains the appearance of equivalent formulae for the effective properties, containing refractivity instead of dielectric properties.

and it has come to be known as the Clausius-Mossotti's one. But several years before Clausius' publication, an analogous formula in conductivity had been given by Maxwell [MAj], whose reasoning will be presented below.

Note also that L. Lorenz in three papers between 1869 and 1880 considered optical problems, concerned with propagation of electromagnetic waves ("optical vibrations" as he called them) [LOc]. He assigned a refractive index to each molecule that differs from that of the surrounding medium and then employed a scheme which resembled very much what is now called the Coherent Potential Approximation. That is why the local field and its expression, to be discussed in an appropriate context in Section 1.5.5.1, is often called Lorenz-Lorentz's field.

1.1.3.3 Maxwell

In his famous treatise [MAj] Maxwell addressed in passing the problem of predicting the overall behavior of a dispersion of spheres, immersed into a matrix of different conductivity. We shall repeat here his elegant and simple reasoning, since it contains a number of basic ideas and drawbacks that have kept reappearing in the later works for a long period afterward.

The basic building block in Maxwell's study is the single sphere field. Let a single spherical inhomogeneity \mathcal{V}_a , located at the origin, be immersed into an unbounded matrix. Let the applied far-field have a constant and prescribed gradient, i.e. $\theta^\infty(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}$. The temperature field, $\theta(\mathbf{x})$, is governed then by the equation:

$$\begin{aligned} \nabla \cdot (\kappa(\mathbf{x}) \nabla \theta(\mathbf{x})) &= 0, \quad \theta(\mathbf{x}) \rightarrow \mathbf{G} \cdot \mathbf{x} \text{ as } |\mathbf{x}| \rightarrow \infty, \\ \kappa(\mathbf{x}) &= \kappa_1 + [\kappa] h_a(\mathbf{x}), \quad [\kappa] = \kappa_2 - \kappa_1, \end{aligned} \quad (1.7)$$

where $h_a(\mathbf{x})$ is the characteristic function of the sphere \mathcal{V}_a , κ_1 and κ_2 are the conductivities of the matrix and of the sphere, respectively, see Eqs. (1.5) and (1.6).

Since $\kappa(\mathbf{x})$ is a step-constant function, the field $\theta(\mathbf{x})$ should be a harmonic function both inside and outside the sphere; on the sphere surface, $|\mathbf{x}| = a$, it should be continuous together with the normal component of the heat flux:

$$\kappa_2 \frac{\partial \theta}{\partial r} \Big|_{r=a-0} = \kappa_1 \frac{\partial \theta}{\partial r} \Big|_{r=a+0}, \quad (1.8)$$

as it follows directly from (1.7); here $r = |\mathbf{x}|$ is the radial coordinate, a is the sphere's radius.

The solution of Eq. (1.7) depends linearly on the far-field gradient \mathbf{G} . Together with the obvious geometrical symmetry, this suggests to look for the needed solution in the form

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \nabla \varphi(r). \quad (1.9)$$

Since $\theta(\mathbf{x})$ is harmonic, Eq. (1.9) implies

$$\Delta \theta(\mathbf{x}) = \mathbf{G} \cdot \nabla \Delta \varphi(r) = 0, \quad \text{i.e.} \quad \Delta \varphi(r) = \text{const},$$

and hence

$$\varphi(r) = \frac{1}{2} C' r^2 - C'' a/r + \text{const}. \quad (1.10)$$

Obviously, the additive constant in the last formula does not influence the solution (1.9). Inside the sphere $C'' = 0$, in order to have a bounded everywhere solution there, so that

$$\theta(\mathbf{x}) = C' \mathbf{G} \cdot \mathbf{x}, \quad |\mathbf{x}| < a. \quad (1.11)$$

Outside the sphere $C'' = 1$, in order to meet the far-field condition in Eq. (1.7), and hence

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} \left(1 - C'' (a/r)^3 \right), \quad |\mathbf{x}| > a. \quad (1.12)$$

The continuity conditions for $\theta(\mathbf{x})$ and for the normal flux at $|\mathbf{x}| = a$, see Eq. (1.8), yield

$$C' = 1 + C'', \quad \kappa_2 C' = \kappa_1 (1 - 2C''),$$

as it follows from Eqs. (1.11) and (1.12), and also from the simple formula

$$\frac{\partial \theta}{\partial r} = \mathbf{e}_r \cdot \nabla \theta(\mathbf{x}) = \mathbf{G} \cdot \nabla \nabla \varphi(r) \cdot \mathbf{e}_r = \varphi''(r) \mathbf{G} \cdot \mathbf{e}_r, \quad (1.13)$$

$\mathbf{e}_r = \mathbf{x}/r$, $r = |\mathbf{x}|$, which holds for any function of the form (1.9). The solution of the single inclusion problem (1.7) therefore reads

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} \begin{cases} \gamma, & \text{if } |\mathbf{x}| < a, \\ 1 - \beta (a/r)^3, & \text{if } |\mathbf{x}| > a, \end{cases} \quad (1.14)$$

with the constants

$$\beta = \frac{[\kappa]}{\kappa_2 + 2\kappa_1}, \quad \gamma = 1 - \beta = \frac{3\kappa_1}{\kappa_2 + 2\kappa_1}. \quad (1.15)$$

Remark 1.1 *In Section 1.4.2 we shall find the solution of Eq. (1.7) inside the sphere in a much simpler way, which works equally well for an ellipsoidal inhomogeneity also. In Maxwell’s considerations one needs, however, the field $\theta(\mathbf{x})$ outside the sphere, so that a more lengthy analysis is required.*

Remark 1.2 *The formula (1.14) shows that if the temperature gradient at infinity is constant, the same holds true for this gradient inside a spherical inhomogeneity. This is a particular case of a more general statement in which the sphere is replaced by an ellipsoidal inhomogeneity. A similar statement holds for the elastic inhomogeneity problem, see Section 1.4.4.*

With the single-sphere solution found, we can go back to Maxwell’s analysis. Consider a large sphere \mathcal{V}_A of the radius A and conductivity κ_1 , containing N identical and nonoverlapping small spheres of conductivity κ_2 . (“Large” means here that $A \gg a$, where a is the radius of the small spheres.)

Immerse the sphere \mathcal{V}_A into a homogeneous medium possessing the same conductivity κ_1 as that of the matrix. “Sit down” at the point M , far away from the center O of the sphere, i.e. imagine $R \gg A$, where $R = |OM|$. Assume again that the temperature gradient \mathbf{G} at infinity is constant. The presence of the inhomogeneous sphere \mathcal{V}_A will disturb the field $\mathbf{G} \cdot \mathbf{x}$ that would have existed in the homogeneous medium of conductivity κ_1 at its absence. We shall evaluate this disturbance in *two* different ways.

First, let us consider each small sphere within \mathcal{V}_A as a single and pretend there are no other small spheres around it. Then, according to Eq. (1.14), the disturbance, caused by any such sphere, is $-\beta a^3/R^3$, and summing up all of them, gives

$$-N\beta \frac{a^3}{R^3} = -N \frac{a^3}{R^3} \frac{\kappa_2 - \kappa_1}{\kappa_2 + 2\kappa_1}; \quad (1.16)$$

recall that the small spheres within \mathcal{V}_A are located practically at one and the same distance R from our observation point M , since $R \gg A$.

Second, “looking” at the big sphere \mathcal{V}_A from a great distance, we can “homogenize” it, neglecting its heterogeneous internal structure and replacing it by a homogeneous sphere possessing a certain unknown effective conductivity κ^* . The disturbance, caused by such a

homogeneous sphere at the point M , is

$$-\beta^* \frac{A^3}{R^3} = -\frac{A^3}{R^3} \frac{\kappa^* - \kappa_1}{\kappa^* + 2\kappa_1}, \quad (1.17)$$

as it follows again from Eq. (1.14).

It is natural now to equate the disturbances (1.16) and (1.17), calculated in these two different ways (which just reflects the above mentioned idea of “homogenization”—replacement of the heterogeneous sphere \mathcal{V}_A by an equivalent homogeneous one; *equivalent* in the sense that it behaves (i.e. disturbs) the temperature field in *exactly* the same way). This results in the equation

$$-N \frac{a^3}{R^3} \frac{\kappa_2 - \kappa_1}{\kappa_2 + 2\kappa_1} = -\frac{A^3}{R^3} \frac{\kappa^* - \kappa_1}{\kappa^* + 2\kappa_1},$$

or

$$\frac{\kappa^* - \kappa_1}{\kappa^* + 2\kappa_1} = \phi_2 \beta, \quad \phi_2 = N \frac{V_a}{V_A} = N \frac{a^3}{A^3}, \quad (1.18)$$

so that ϕ_2 is the volume fraction of the spheres in \mathcal{V}_A ; $V_a = \frac{4}{3}\pi a^3$ and $V_A = \frac{4}{3}\pi A^3$ are the volumes of the respective spheres. From (1.18) it follows

$$\frac{\kappa^*}{\kappa_1} = \frac{1 + 2\beta\phi_2}{1 - \beta\phi_2}, \quad (1.19)$$

and this is *exactly* the formula, known now as Clausius-Mossotti’s (in dielectric context) or Maxwell’s (in conductivity context), and also Lorenz-Lorentz’s (in refractivity context, see the footnote on page 10). Having derived (1.19), Maxwell remarked that it “*may be obtained in other ways, but that here given involves only repetition of the result already obtained for a single sphere*” [MAj, Section 314].

Due to the above explained reasons, and to the fact that we shall deal mainly with conductivity problem in the sequel, we shall refer to (1.19) as Maxwell’s formula. Its derivation possesses the obvious drawback that each sphere is considered as single, so that the result (1.19) is strictly valid *only* in the dilute limit $\phi_2 \ll 1$:

$$\frac{\kappa^*}{\kappa_1} = 1 + 3\beta\phi_2 + o(\phi_2), \quad (1.20)$$

when the spheres are sparse. This fact was entirely clear to Maxwell himself (see the same Section 314 of his *Treatise*) and to his contemporaries. Lord Rayleigh [RAa], in order to check the exactness and

applicability of (1.19) for higher values of ϕ_2 , considered a special kind of internal constitution, assuming that the inclusions are spheres or cylinders, forming a regular periodic array. (A vast number of studies concerning the properties of periodic media were initiated by this classical paper.) The basic Rayleigh's conclusion was that (1.19) does hold for dilute to moderate concentrations ϕ_2 , but for closer packing of spheres and cylinders, considerable deviations from the predicted values are present.

The evaluation of the terms of higher orders in Eq. (1.20), e.g. the one proportional to ϕ_2^2 , requires already that spheres' interactions be taken into account. If it is done properly, then the spatial statistics of the sphere' distribution should enter the result. The appropriate problem appears very hard and had to wait exactly 100 years after Maxwell, when Jeffrey [JEa], in 1973, derived the first exact formula for the successive ϕ_2^2 -coefficient in the power expansion (1.20).

1.1.3.4 Einstein

The dawn of the 20th century witnessed the emergence of some new micromechanical problems whose motivation was already different from the mainly electrical "preoccupation" of the previous century (a notable exception was the classical Voigt quest for the effective elastic properties of a polycrystal [VOa]). In a pioneering paper on viscosity of dilute suspensions Einstein [EIa], in his PhD dissertation, addressed the question of experimental measurement of the size of molecules. His simple and innovative reasoning may be summarized as follows.

Consider a known amount of molecules, n , per unit volume of a solvent. The molecules are identical, and each one is imagined as a rigid sphere of an unknown radius a . Thus there exists a volume concentration $\phi_2 = nV_a = n\frac{4}{3}\pi a^3$ of particles in the solvent, i.e. a liquid suspension is to be studied. Let the liquid be Newtonian, of viscosity μ_1 . The presence of the rigid spheres will undoubtedly make the suspension more "viscous," so that it will possess a certain gross macroscopical viscosity μ^* . The micromechanical problem consists in evaluating μ^* , provided μ_1 and the volume fraction ϕ_2 of the molecules are known. Einstein solved this problem for slow motions (in the Stokesian approximation, that is) and in the dilute case, when $\phi_2 \ll 1$ and hence the many-particle interactions can be

neglected. Each sphere (molecule) can be then considered as single, immersed into a given (shear, to be more specific) flow of the fluid at infinity. The presence of the sphere, perturbing the flow, will increase the energy dissipation, by a certain quantity Δ , proportional to the spheres' volume V_a . Technically, the correct formula for Δ was the core of Einstein's calculations. Since the interactions are neglected, the total dissipation's increase will be $n\Delta$, i.e. n times higher. This increase, from a macroscopical point of view, can be attributed to the change of the gross viscosity of the suspension, which has the needed value μ^* , and this fact led him to the now famous formula

$$\frac{\mu^*}{\mu_1} = 1 + 2.5\phi_2 + o(\phi_2), \quad (1.21)$$

named after him.⁶ Though Einstein reasoning is based on some simple solutions of the Stokes equations, his derivation is quite technical and will be omitted here. The classical formula (1.21) will be derived in Section 1.5.2 below as a particular case of a more general result (see Remark 5.6).

The term $o(\phi_2)$, added in the right-hand side of Eq. (1.21), underlines the fact that it is strictly valid, similarly to the Maxwell's one (1.19), *only* in the dilute case $\phi_2 \ll 1$, when the spheres' interactions can be totally neglected.

Applying the formula Eq. (1.21) for sugar solutions and using some viscosimetric data, Einstein was able to obtain experimentally the volume concentration $\phi_2 = nV_a$ of the sugar molecules; for a given n , it led him to a certain value of their radius a which turned out to represent reasonable approximation of the latter. For our purposes, however, much more interesting is the micromechanical problem, posed by Einstein, namely, how to evaluate a macroscopic property (viscosity), using the available microscopic information, i.e., in the dilute case, the viscosity of the solvent and the volume fraction of the particles.

1.1.3.5 Smoluchowski

Another classical micromechanical problem was introduced in 1916 by Smoluchowski in his "Three papers on diffusion, Brownian motion

⁶As a matter of fact, Einstein introduced and used the so-called "energy" definition of the effective properties; see Section 1.2.4 below.

and coagulation in colloid solutions” [SMa]. There he considered, in particular, a dilute array of fixed spheres that absorb a species diffusing around. The question was what is the mean rate of absorption in such a system of spheres, provided the concentration is kept constant at infinity.

Since the array is dilute, each sphere (of the radius a) can be treated as alone, located at the origin. In the steady-state limit the species concentration $c(\mathbf{x})$ is governed by the equation:

$$\Delta c(\mathbf{x}) = 0, \quad c(\mathbf{x}) \Big|_{r=a} = 0, \quad c(\mathbf{x}) \xrightarrow{r \rightarrow \infty} c_0, \quad (1.22)$$

whose solution is obvious

$$c(r) = c_0 \left(1 - \frac{a}{r} \right), \quad r \geq a. \quad (1.23)$$

The flux of the diffusing species within the sphere is

$$- \int_{r=a} \mathbf{j}(\mathbf{x}) \cdot \mathbf{e}_r \, dS,$$

where $\mathbf{j}(\mathbf{x}) = -D\nabla c(\mathbf{x})$ is the local flux vector (according to Fick’s law) and D is the diffusing coefficient. Employing Eq. (1.23) gives the value $4\pi a D c_0$ for this flux. If n is the number density of the spheres, the total flux K due to all spheres, i.e. the total rate of absorption, is n times bigger (recall the dilute assumption). Hence

$$K = k_s^2 c_0, \quad k_s^2 = 4\pi a n D = \frac{3}{a^2} \phi_2 D; \quad (1.24)$$

similarly to the foregoing analysis of fluid dispersions, $\phi_2 = nV_a$ is the volume fraction of the spheres.

Thus there is a balance between creating diffusing species (in order to keep its concentration, c_0 , at infinity fixed) and its “removal” due to the spherical “traps” or “sinks.” The proportionality coefficient between c_0 and this removal rate, K , is just the so-called *effective reaction-rate constant* or the *effective absorption coefficient*, denoted by k^{*2} :

$$K = k^{*2} c_0, \quad k^{*2} = k_s^2 + \mathcal{O}(\phi_2). \quad (1.25)$$

(k^{*2} is also called *trapping constant* or *sink strength*.)

Similarly to the foregoing Einstein’s formula (1.21), $\mathcal{O}(\phi_2)$ is added in the right-hand side of Eq. (1.25) to underline the fact that the

Smoluchowski's value k_s^2 is the dilute approximation of the effective sink strength, strictly valid *only* when the spheres' interactions are totally neglected.

Smoluchowski's paper initiated a broad and extensive research activity, concerned with the so-called diffusion-controlled reactions—chemical events whose rate decisively depends on the transport processes, like diffusion, in a solution of reactant entities. For more details and different points of views and interpretations, concerning the ideas, results and basic references in this important field the reader is referred to the papers [FEa], [TAa], or to the survey of Calef and Deutch [CAa]. For our aims here much more interesting, once again, is the micromechanical problem, posed by Smoluchowski, namely, how to evaluate a macroscopic property (the effective rate constant now), using the available microscopic information, i.e. in the dilute case, the volume fraction of the spheres.

1.1.4 Outline of the Survey

A number of the simplest ideas, methods and results, concerning homogenization procedures for heterogeneous media, are collected in the present survey, with no pretense to give a full exposition. The aim is much more modest—to provide a certain basic reading and a general picture for a newcomer to gain some necessary knowledge, before proceeding to more specific aspects and (extremely voluminous) specialized literature. Another aim lies also in underlying the common nature and unity of the problems and approaches, spread through many different communities, to mention only pure mathematics (homogenization of differential equations with periodic and random coefficients), solid mechanics (composite materials), hydromechanics (liquid dispersion and emulsions, flows through porous media), geophysics (micromechanics of rocks), chemical physics (diffusion-absorption reactions), and so on and so forth. Though the context, the terminology, the way of thinking and “language” may widely vary, behind many of the central, for these fields, problems lies *one and the same fundamental quest* about the “micro-macro” interconnection.

The list of references, though extensive, by no means pretends to be exhaustive. It includes some (but not all) of the basic works in the fields and may provide a certain guide where to find further details and references for interested readers. We have tried to mention as well some of the earlier and perhaps not very well-known works in

this field to demonstrate that the basic and classical ideas are old and, typically for any classic, have been rediscovered many a time.

Only static behavior and static approaches will be discussed here. A thorough and critical discussion of somewhat similar methods, using wave phenomena and, in particular, features of scattered fields by single inclusions in a particulate medium, can be found in Berryman's papers [BE_m], [BE_n].

The volume-average approach is used throughout, which may explain the word *elementary* in the title. Though this approach possesses certain inherent inconsistencies at a closer look (underlined in due course below), it seems more appealing to the author for introductory purposes and for a broader audience. The word *elementary* underlines also the fact that in recent decades heterogeneous media have been studied by means of new and much more refined methods. The statistical modelling has already been mentioned, together with the book [BE_i] (see also [KRf]). The methods, based on various homogenization procedures (such as two-scale expansions, G -convergence and so on), have received special attention; see, e.g. the books [SAa] or [ZHa]. The modelling aspects, concerned with determination of "optimal" micro-structures, should be specially mentioned as well. The appropriate problems, ideas, and results in this field can be found in [MIg]. The author hence believes that in view of the recent extensive research activity, combining new mathematical tools and approaches, the reasoning and the results, collected in the present survey, indeed deserve to be called *elementary*.

The basic notions and definitions are introduced in Section 1.2; there, as in the rest of the paper, the scalar conductivity context is first used for illustration. The reason is that, being simpler formally, it allows one to concentrate on the basic problems, unshaded by technical details that may appear in a similar elastic context. There are two central results of the Section: (i) the equivalence of the energy definition of the effective properties to the usual ones, under homogeneous boundary conditions; (ii) the Willis result of consistency, stating that the effective conductivity and resistivity are the inverse of each other. Moreover, the Willis reasoning, reproduced in a simplified situation here, clarifies the special role of the homogeneous boundary conditions and proclaims their "extremum" properties.

Some of the "evergreens" of the theory of heterogeneous media

are collected in Section 1.3. This is the perturbation theory for a weakly inhomogeneous materials, as initiated by Brown in 1955 [BRd]. The Bergman formula is then derived [BEk], which interconnects the derivatives of the effective conductivity with respect to the properties of the constituents with the mean “energies,” accumulated within the latter. Only one of the simpler applications of this important formula is exploited—the beautiful Matheron derivation [MAi] of the Hashin-Shtrikman estimates on the effective conductivity, without invoking the original variational arguments of Hashin and Shtrikman [HAk]. These bounds hold under the sole assumption that the material is macroscopically isotropic. The Hashin assemblage [HAe] is then constructed to demonstrate that the bounds are sharp, in the sense that they *cannot* be improved. The Beran’s bounds are then derived and simplified, after Torquato and Milton; the appearance of three-point statistical parameters there indicates that the effective properties depend in general on *all* details of the internal structure, as reflected by the appropriate “multipoint” characteristics (correlations) of a heterogeneous medium. The cross-property relations and their “philosophy” are briefly discussed as well; the original derivation of the first such relation, due to Levin [LEa], is supplied: it interconnects *exactly* the effective bulk modulus and thermal expansion coefficient.

In Section 1.4 the single particle problem is discussed in various contexts. The well-known Eshelby result [ESa] is first proved, stating that the temperature gradient (or the strain) within an ellipsoidal inhomogeneity immersed in a homogeneous matrix is constant provided the applied gradient (or strain) at infinity is constant. The reasoning here is simplified, as compared to the original Eshelby’s one, and follows, as a matter of fact, Wu [WUa].

The aim of Section 1.5 is to show how various “repetitions” (to cite again Maxwell [MAj, Section 314]) of the single-inclusion solution of Section 1.4 can be systematically utilized in order to derive the basic and most widely used approximate (static) models for predicting the effective properties of particulate media, like self-consistent, differential scheme and effective field. The starting point are the “concentration” factors, introduced in Section 1.2, and the representations, due to Reynolds and Hough [REb] and Hill [HIb] of the effective properties, through these factors. Each approximation then corresponds to a certain qualitative and intuitively appealing replacement of a con-

centration factor by a quantity that stems out from the appropriate solution for a single inhomogeneity.

Section 1.6 demonstrates, after Hershey [HEb] and Kröner [KRd], the application of the self-consistent arguments for predicting the effective elastic moduli of polycrystals. As an illustration, the simplest case of cubical symmetry of grains is treated at some length.

The survey is a (considerably) extended version of the course on composite and heterogeneous media, read by the author in the last years for graduate students in the Faculty of Mathematics and Informatics at the “St. Kliment Ohridski” University of Sofia. (A number of topics were included also in the author’s lectures presented in 1994 at the Department of Engineering Sciences of the Istanbul Technical University and, in 1997, in the Department of Mathematics of Torino Polytechnics.) As a consequence, the exposition is quite detailed with no “incantations” of the kind “it is easily seen . . .”. Besides a natural curiosity, nothing more than a basic knowledge of differential equations, continuum mechanics and tensor calculus is required from a reader.

As a rule, the bold-face lower-case letters e , \mathbf{x} , \mathbf{y} , etc., are used for vectors. The upper-case such letters \mathbf{A} , \mathbf{K} , etc., are reserved for second-rank tensors, the shadow symbols \mathbb{A} , \mathbb{L} , etc., denote fourth-rank tensors. Dyadic notations are used, e.g. $\mathbf{xy} = \mathbf{x} \otimes \mathbf{y}$ is the dyadic product of the vectors \mathbf{x} and \mathbf{y} . The dot stands for a contraction with respect to one pair of indices, and the colon—with respect to two pairs, say,

$$(\mathbf{A} \cdot \mathbf{B})_{ij} = A_{i\alpha} B_{\alpha j}, \quad (\mathbb{A} : \mathbb{B})_{ijkl} = A_{ij\alpha\beta} B_{\beta\alpha kl},$$

in a Cartesian system, with the summation convention adopted throughout.

1.2 The Homogenization Problem

The simplest point of view, already introduced and briefly discussed on the examples in the previous Section, is that a heterogeneous medium behaves macroscopically in the same way, as do its constituents, but with different, *effective*, values of the appropriate material constants. In the present Section we shall try to put this point

of view on a clearer framework, introducing and analyzing the definition of the effective properties.

1.2.1 The Representative Volume Element

A basic notion in micromechanics is the *representative volume element* (RVE). Though it can be more rigorously defined, see e.g. [DRa], it is appropriate to be imagined in the following manner [HIb]. This is a volume which is small enough from a macroscopical point of view and could be thus treated as a typical “point” of the heterogeneous continuum under study. On the other hand, it should be large enough in the microscopical scale, in order to contain a large number of single inhomogeneities and therefore to be indeed typical “representative” for the microstructure of the solid. A more detailed discussion of RVE’s, together with certain criteria how to identify them, can be found in the book [NEa, Chapters 1.3 and 2.5.4].

It is noted that the notion of RVE (as well as the volume averaging procedure to be used in the sequel) was clearly and vividly described already in the classical Lorentz’ book [LOb, Section 113]. The author introduces there the mean value $\bar{\phi}$, over a ball \mathcal{S} , of a microscopically fluctuating quantity ϕ , and adds that the size of the ball should be neither too big nor too small, in order to get a meaningful macroscopic characterization of ϕ . Lorentz’s comments on the words “too big” and “too small,” that followed in the same Chapter, is just what is now understood as a RVE.

The foregoing “definition” of a RVE will undoubtedly leave unhappy any reader with a more rigorous taste. It should be pointed out, however, that this notion is very convenient on a heuristic and elementary level of consideration, pursued in this survey, and allows us to introduce and develop the basic ideas and some of the simplest techniques of micromechanics, in general, and of mechanics of composites, in particular. A more rigorous approach, say, for random media, does not need the notion of RVE at all. Note that for periodic media the RVE is unambiguously defined (this is simply the typical unit cell of the structure). It is to be noted also that our RVE here is just the well-known “material point” of a continuous medium—the basic notion, which lies in the foundation of continuum mechanics. The only difference is the size of inhomogeneities: for the latter they often correspond to molecular or atomistic scales. For heterogeneous solids this size is defined by the dimensions of a typical inclusion or

of a monocrystal (in a polycrystalline aggregate).

The heterogeneous media considered here can be thus characterized, after Hashin [HAI], in the following manner. It is possible to distinguish within them representative volume elements which are small macroscopically. Their typical dimension defines the so-called *mini-scale*. A RVE consists of a big amounts of much smaller inhomogeneities (inclusions, monocrystals, etc.), whose dimension defines the *micro-scale*. The composite medium itself consists of many RVE; its size defines, in turn, the *macro-scale*. For the very idea of homogenization to be sensible and to produce widely applicable results, the following inequalities between the above defined three length scales should hold:

$$\text{MICRO} \ll \text{MINI} \ll \text{MACRO} . \quad (2.1)$$

After Hashin [HAI], we shall call (2.1) the *MMM principle*.

Note that though general, the violation of the MMM principle in certain approximate homogenization schemes *does not imply* that the resulting predictions are useless or should be immediately rejected. It rather indicates that the internal structures, for which the schemes may be applicable and useful, have little in common with the simplified models (like dispersions of identical particles), utilized when deriving the appropriate approximations for the effective properties (see Section 1.5.3.1 below).

Remark 2.1 *The MMM principle can be traced back as far as the Poisson’s 1829 Mémoire [POc, p. 149], where he wrote: “The molecules are so small and so close to one other that a portion of a body containing an extremely large number of them can be still supposed to be extremely small and to have an insensibly small volume.” (translation and citation after Arnold [ARb, p. 364]). As pointed out by Arnold in the same paper, this statement is crucial to Poisson’s conception of matter. In our context, the latter is but a heterogeneous medium (with the “molecules” treated as certain inhomogeneities), which we macroscopically observe and study as homogeneous on this level.*

Remark 2.2 *The fact that only two length scales—micro and mini—are considered hereafter, besides the macroscopic one, means that one more assumption is tacitly adopted: namely, that the applied external field is either macroscopically homogeneous or varies slowly. If*

this field varies rapidly, as it is the case with the wave propagation problems, when the wave-length is of the order of the micro-length ℓ , the situation drastically changes. The homogenization can still be performed (though ensemble averaging should be used from the very beginning), but the macroscopic equations will be nonlocal. Any discussion of nonlocality goes, however, far beyond the scope of the present survey. It suffices to say only that in this case the stress, e.g. in a “point” would depend on the strain within the entire body through a certain integral operator. For details, discussion and references, the reader is referred to the book [KUa], see also [WIE].

The position of a typical mini-element (a RVE) is identified by \mathbf{X} , so that all continuum quantities like temperature, flux, stress and strain fields, etc., are functions of \mathbf{X} . (Hereafter, stationary problems will be only discussed, and hence the time t is not present.) To distinguish these fields from the same ones within the RVE which exemplifies the internal structure of a typical continuum’s “point,” the continuum fields are referred to as macro-fields, and those within a RVE as micro-fields, respectively. That is, instead of saying, for example, “the temperature within the continuum” or “the temperature field within the RVE, that corresponds to the particle \mathbf{X} ,” the expressions macrotemperature field and microtemperature field are used. In a similar manner, the continuum displacement, mass-density, strain, stress, and other physical quantities are identified by an appropriate use of the prefix “macro,” and those within a RVE by the prefix “micro.” Again the analogy with the typical reasoning, contained at the opening pages of textbooks on continuum mechanics, can be easily observed: The only difference lies in the interpretation and in the size of the “material point”—the RVE in our case.

The physical quantities of interest on the micro-level, i.e. within the RVE, depend also on the local coordinate \mathbf{x} , e.g. the temperature $\theta = \theta(\mathbf{X}; \mathbf{x})$ varies *both* on macro- and micro-levels. (The dependence of both macro- and micro-coordinates \mathbf{X} and \mathbf{x} indicates that the internal fields in the medium vary, in general, in different ways in different RVE’s.) The connection between the macro- and micro-quantities is supplied by the volume averaging, with respect to the micro-coordinate \mathbf{x} , e.g.

$$\overline{\theta(\mathbf{X})} = \frac{1}{V} \int_{\mathcal{V}} \theta(\mathbf{X}; \mathbf{x}) \, d\mathbf{x}, \quad \text{etc.}, \quad (2.2)$$

where \mathcal{V} is the RVE, “attached” to the macro-point \mathbf{X} , and $V = \text{vol } \mathcal{V}$.

Since the point \mathbf{X} spans the body, the quantities like $\overline{\theta(\mathbf{X})}$ in Eq. (2.2) are called *moving averages*. Such averages play a central role in the elementary theory of effective properties, developed and discussed below.

In what follows the analysis will be restricted to the important class of statistically homogeneous materials. In the terminology of moving averages it means, roughly speaking, that the macroscopic properties of almost all RVE’s (more precisely, except those near the macroscopic boundary of the solid) are one and the same, see [Haf] and [NEa] for more details and comments.

The assumption of statistical homogeneity allows us to deal in what follows with a single RVE, \mathcal{V} . The latter indeed will be then *representative*, in the sense that it will possess the same gross properties as all of the rest of such elements. These properties will then coincide with those of the medium as a whole. That is why the words RVE, the volume \mathcal{V} and the medium will be used hereafter interchangeably as synonyms.

In most of the cases, treated below, we shall assume that the medium is statistically isotropic as well; again, without entering a longer discussion, we shall only point out that the latter means that the macroscopic properties under study are independent of direction.

1.2.2 Definition of the Effective Conductivity

Let \mathcal{V} be a RVE. Consider the heat propagation problem (1.5) in \mathcal{V} , with the boundary condition

$$\theta(\mathbf{x}) \Big|_{\partial\mathcal{V}} = \mathbf{G} \cdot \mathbf{x}, \quad (2.3)$$

$\partial\mathcal{V}$ is the boundary of \mathcal{V} . If the RVE is homogeneous, then $\theta(\mathbf{x}) \equiv \mathbf{G} \cdot \mathbf{x}$, $\forall \mathbf{x} \in \mathcal{V}$, and thus $\overline{\nabla\theta} \equiv \mathbf{G}$. That is why (2.3) will be called a *homogeneous boundary condition*.

For a heterogeneous RVE, the field $\theta(\mathbf{x})$ fluctuates inside \mathcal{V} . However, the boundary conditions (2.3) yield that

$$\overline{\nabla\theta} = \mathbf{G}, \quad (2.4)$$

as if the volume were homogeneous. This fact is a consequence of a more general statement, see [HAh, Section 3.1] or [NEa], which we shall first formulate in the simpler scalar case:

Lemma 2.1 *Whatever the composition and microstructure of the RVE, the volume average of the temperature gradient is completely determined by the temperature of the boundary $\partial\mathcal{V}$.*

Proof. Let $\theta(\mathbf{x})$ be a temperature field in \mathcal{V} , attaining prescribed boundary values $\theta^0(\mathbf{x})$. Using the Gauss theorem, we have

$$\begin{aligned}\overline{\nabla\theta} &= \frac{1}{V} \int_{\mathcal{V}} \nabla\theta(\mathbf{x}) \, d\mathbf{x} \\ &= \frac{1}{V} \int_{\partial\mathcal{V}} \mathbf{n}\theta(\mathbf{x}) \, dS = \frac{1}{V} \int_{\partial\mathcal{V}} \mathbf{n}\theta^0(\mathbf{x}) \, dS,\end{aligned}\tag{2.5}$$

where \mathbf{n} is the outward unit vector to the boundary $\partial\mathcal{V}$. Eq. (2.5) shows that the boundary values $\theta^0(\mathbf{x})$ do specify the volume average $\overline{\nabla\theta}$ uniquely. \square

In particular, if $\theta^0(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}$, Eq. (2.5) implies

$$\begin{aligned}\overline{\nabla\theta} &= \frac{1}{V} \int_{\partial\mathcal{V}} \mathbf{n}\mathbf{G} \cdot \mathbf{x} \, dS \\ &= \frac{1}{V} \int_{\mathcal{V}} \nabla(\mathbf{G} \cdot \mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \mathbf{G} \cdot \int_{\mathcal{V}} \nabla\mathbf{x} \, d\mathbf{x} = \mathbf{G},\end{aligned}\tag{2.6}$$

which proves (2.4) (having used once more the Gauss theorem and the fact that $\nabla\mathbf{x} = \mathbf{I}$, where \mathbf{I} is the unit second-rank tensor).

Consider now Eq. (1.5) with respect to the temperature field, i.e.

$$\nabla \cdot (\kappa(\mathbf{x})\nabla\theta(\mathbf{x})) = 0,\tag{2.7}$$

with the boundary condition (2.3). Since $\kappa(\mathbf{x}) > 0$, it can be easily shown that the BVP problem (2.7), (2.3) possesses a solution, $\theta(\mathbf{x})$, which is unique. The latter allows us to evaluate the mean heat flux over the RVE under study

$$\mathbf{Q} = \bar{\mathbf{q}} = \overline{\kappa(\mathbf{x})\nabla\theta(\mathbf{x})} = \frac{1}{V} \int_{\mathcal{V}} \kappa(\mathbf{x})\nabla\theta(\mathbf{x}) \, d\mathbf{x}.\tag{2.8}$$

Due to the obvious linearity of the boundary-value problem (2.3), (2.7) with respect to \mathbf{G} , the vector \mathbf{Q} is a linear function of \mathbf{G} , i.e.

$$\mathbf{Q} = \mathbf{K}^* \cdot \mathbf{G},\tag{2.9}$$

where \mathbf{K}^* is the second-rank tensor of *effective conductivity* of \mathcal{V} . In the statistically isotropic case, this tensor is spherical, so that (2.9) reduces to

$$\mathbf{Q} = \kappa^* \mathbf{G}, \quad (2.10)$$

with κ^* being the *effective* (or *overall*, or *macroscopic*) *conductivity* of the volume \mathcal{V} .

Eq. (2.9) means that we replace the micro-inhomogeneous volume \mathcal{V} by a homogeneous one, with conductivity \mathbf{K}^* , which, from a microscopical point of view, “reacts” in the same way. Thus, if we are not interested in detailed microscopic fields within the RVE, but rather in the macroscopically measured quantities like the volume averages $\bar{\mathbf{q}}$, $\overline{\nabla\theta}$, etc., we can *homogenize* \mathcal{V} , i.e. treat it as a homogeneous entity possessing the overall conductivity κ^* . The problem then consists in evaluating \mathbf{K}^* making use of appropriate information about the microstructure of \mathcal{V} . This is a typical and very difficult problem of micromechanics of heterogeneous and composite media.

The fundamental reason that makes the evaluation of the effective properties so difficult, can be well seen from the very structure of Eq. (2.7). At first glance, the BVP (2.7), (2.3) looks innocuous, resembling the ones treated in the basic books on PDE’s. In these books, however, the emphasis lies on the dependence of the solution upon the boundary data, which is obviously linear. Here the boundary condition is fixed, and one should find the solution $\theta(\mathbf{x})$ for given coefficients $\kappa(\mathbf{x})$; the dependence of $\theta(\mathbf{x})$ upon the latter is already *nonlinear*, as first pointed out by Kraichnan [KRa] (in a physically entirely different context though). This gives rise to very serious mathematical complications, *common* for all problems concerning heterogeneous media and their homogenization. Typical and very important among them is the fact that even the mean value of the solution, like the one in Eq. (2.8), depends on *all* details of the internal structures of the medium. More persuasive and specific arguments in support of this statement will be given in Section 1.3.1.3 below, on the example of a weakly inhomogeneous medium.

Remark 2.3 *If, by chance, the temperature gradient is constant within \mathcal{V} , i.e. $\theta(\mathbf{x}) \equiv \mathbf{G} \cdot \mathbf{x}$, if $\mathbf{x} \in \mathcal{V}$, the effective conductivity κ^* is exactly the mean $\bar{\kappa}$ of the constituents’ conductivities. Hence*

for an N -phase medium

$$\kappa^* = \bar{\kappa}, \quad \bar{\kappa} = \sum_{i=1}^N \phi_i \kappa_i, \quad (2.11)$$

as easily seen from Eqs. (2.8) and (2.10); here $\phi_i = V_i/V$ is the volume fraction of the i th constituent that occupies the volume $\mathcal{V}_i \subset \mathcal{V}$; κ_i is its conductivity, $i = 1, \dots, N$.

The assumption that the temperature possesses a constant gradient within the medium was adopted, as a matter of fact, by Voigt [VOa], in his study of elastic moduli of polycrystals (accordingly, he proposed that the strain field is homogeneous within the polycrystalline sample). That is why the approximation (2.11) is called Voigt's and is designated by the superscript 'v', i.e. $\kappa^v = \bar{\kappa}$.

It is noted that a temperature field with a constant gradient does appear in a heterogeneous solid, provided it is a fiber-reinforced or layered material, and the applied macroscopic gradient \mathbf{G} is along the fibers or layers, see Section 1.5.2. If however the gradient \mathbf{G} is perpendicular to the laminae in the layered material, though the volume fractions of the constituents remain the same, its effective conductivity κ^* is already totally different. (In this case it coincides with the Reuss' value, see Eq. (2.18) and Remark 2.2 below.) This simple observation demonstrates that κ^* is indeed sensitive to the internal structure of the medium. As a consequence any theory that tries to predict the effective behavior on the base of the volume concentrations and phases' properties solely can serve, at the best, only as a certain heuristic approximation.

1.2.3 Definition of the Effective Resistivity

Recall that the conduction through a solid can be alternatively studied, choosing as a basic variable the heat flux $\mathbf{q}(\mathbf{x})$ instead of temperature (this is the so-called *dual* formulation). Since $\mathbf{q}(\mathbf{x})$ is divergence-free, $\nabla \cdot \mathbf{q}(\mathbf{x}) = 0$, it can be represented by means of its *vector-potential* $\Phi(\mathbf{x})$:

$$\mathbf{q}(\mathbf{x}) = \nabla \times \Phi(\mathbf{x}), \quad (2.12)$$

where $\nabla \times (\cdot) = \text{curl}(\cdot)$ is the curl of the respective vector field. In turn, the curl of any potential field and, in particular, that of $\nabla\theta(\mathbf{x}) = k(\mathbf{x})\mathbf{q}(\mathbf{x})$, vanishes. Here $k(\mathbf{x}) = 1/\kappa(\mathbf{x})$ is the so-called

resistivity or (inspired by the elasticity terminology), the *compliance field* of the medium.

Hence, the vector potential $\Phi(\mathbf{x})$ satisfies the equation

$$\nabla \times (k(\mathbf{x})\nabla \times \Phi(\mathbf{x})) = 0 \quad (2.13)$$

which is the counterpart of the basic Eq. (2.7) for the temperature field.

Let us prescribe the heat flux on the boundary $\partial\mathcal{V}$

$$q_n \Big|_{\partial\mathcal{V}} = \mathbf{Q} \cdot \mathbf{n}, \quad q_n = \mathbf{q} \cdot \mathbf{n}, \quad (2.14)$$

where \mathbf{Q} is a given vector. For a homogeneous \mathcal{V} , $\mathbf{q}(\mathbf{x}) \equiv \mathbf{Q}$, for all $\mathbf{x} \in \mathcal{V}$, and thus $\bar{\mathbf{q}} = \mathbf{Q}$. That is why the boundary condition (2.14) will be also called *homogeneous* (with respect to flux); it is the counterpart of the homogeneous condition (2.3) for the temperature.

For a heterogeneous \mathcal{V} the field $\mathbf{q}(\mathbf{x})$ fluctuates. However, the boundary condition (2.14) implies that

$$\bar{\mathbf{q}} = \mathbf{Q}, \quad (2.15)$$

as if the volume \mathcal{V} were homogeneous, similarly to Eq. (2.4). This fact is again a consequence of a more general statement, “dual” to Lemma 2.1, see [HAh, Section 3.1] or [NEa], which we shall formulate once again in the simpler scalar case first:

Lemma 2.2 *Whatever the composition and microstructure of RVE, the volume average of the heat flux, at the absence of body sources, is completely determined by its boundary values on $\partial\mathcal{V}$.*

Proof. Let $\mathbf{q}(\mathbf{x})$ be a heat flux field in \mathcal{V} , attaining the prescribed boundary values. Due to the assumed absence of body sources $\nabla \cdot \mathbf{q}(\mathbf{x}) = 0$. In the Cartesian system x_i , $i = 1, 2, 3$, we have, using the Gauss theorem,

$$\begin{aligned} \bar{q}_i &= \frac{1}{V} \int_{\mathcal{V}} q_i(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\mathcal{V}} \delta_{ij} q_j(\mathbf{x}) \, d\mathbf{x} \\ &= \frac{1}{V} \int_{\mathcal{V}} x_{i,j} q_j(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\mathcal{V}} (x_i q_j(\mathbf{x}))_{,j} \, d\mathbf{x} \\ &\quad - \frac{1}{V} \int_{\mathcal{V}} x_i q_{j,j}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\partial\mathcal{V}} x_i q_n(\mathbf{x}) \, dS, \end{aligned} \quad (2.16)$$

and hence $\bar{\mathbf{q}}$ is indeed uniquely specified by the values $q_n |_{\partial\mathcal{V}}$. \square

In particular, let $q_n = \mathbf{Q} \cdot \mathbf{n}$ on $\partial\mathcal{V}$. To check the validity of (2.15), we repeat almost literally the reasoning after Lemma 2.1, see (2.6). Indeed, in virtue of Eq. (2.16),

$$\bar{\mathbf{q}} = \frac{1}{V} \int_{\partial\mathcal{V}} \mathbf{x} q_n \, dS = \frac{1}{V} \int_{\partial\mathcal{V}} \mathbf{x} \mathbf{n} \cdot \mathbf{Q} \, dS = \frac{1}{V} \mathbf{Q} \cdot \int_{\mathcal{V}} \nabla \mathbf{x} \, d\mathbf{x} = \mathbf{Q},$$

which proves (2.15), since $\nabla \mathbf{x} = \mathbf{I}$.

Consider next Eq. (2.13) for the potential $\Phi(\mathbf{x})$, together with the boundary conditions (2.14). This BVP has a solution which is unique in the class of solenoidal fields ($\nabla \cdot \Phi(\mathbf{x}) = 0$). Thus the field $\nabla \times \Phi(\mathbf{x})$ is uniquely defined, and we can evaluate the respective mean temperature gradient

$$\mathbf{G} = \overline{\nabla\theta} = \overline{k(\mathbf{x})\nabla \times \Phi(\mathbf{x})} = \overline{k(\mathbf{x})\mathbf{q}(\mathbf{x})} = k^* \mathbf{Q}. \quad (2.17)$$

The parameter k^* that enters (2.17) is called the *effective* (or *overall*, or *macroscopic*) *resistivity* of the volume \mathcal{V} . (Recall that we have assumed the medium isotropic. Otherwise the constant k^* in (2.17) should be replaced by the appropriate second-rank tensor of effective resistivity.)

The interpretation of Eq. (2.17) is fully similar to that of Eq. (2.10); it means that we “homogenize” the RVE, \mathcal{V} , under study, replacing it by a homogeneous one, with the resistivity k^* . The volume \mathcal{V} , from a macroscopical point of view, will behave then *in the same way* as the heterogeneous one.

Remark 2.4 *If, by chance, the heat flux is constant within \mathcal{V} , i.e. $\mathbf{q}(\mathbf{x}) \equiv \mathbf{Q}$, $\mathbf{x} \in \mathcal{V}$, the effective resistivity is exactly the mean value \bar{k} of the constituents’ resistivities*

$$k^* = \frac{1}{\kappa^*} = \bar{k}, \quad \bar{k} = \sum_{i=1}^N \phi_i k_i = \sum_{i=1}^N \frac{\phi_i}{\kappa_i}, \quad (2.18)$$

as easily seen from Eq. (2.17). Here, similarly to Remark 2.1, ϕ_i and κ_i are the volume fraction and conductivity of the i th constituent, $i = 1, \dots, N$.

The assumption of a constant flux is to be attributed to Reuss [REa] who, similarly to Voigt, studied the elastic moduli of polycrystals (accordingly, he proposed that the stress field is homogeneous

within the polycrystalline sample). That is why the approximation (2.18) is called hereafter Reuss' and is designated by the superscript 'r', i.e. $\kappa^r = (\overline{1/\kappa})^{-1}$.

It is noted that such a constant heat flux field does appear in a heterogeneous solid, provided it represents a layered material, and the applied macroscopic gradient \mathbf{Q} is perpendicular to the layers, cf. Section 1.5.2.

We shall conclude this section with a comment concerning the dual formulation (2.13) of the heat conduction problem. Comparing (2.13) with (2.7), one notices that $\Phi(\mathbf{x})$ is the exact counterpart of the scalar potential $\theta(\mathbf{x})$ (the temperature), with divergence replaced by the curl operator. One may feel tempted to extend this analogy to the boundary conditions as well, and it seems at first glance natural to combine Eq. (2.13) not with (2.14), but rather with the boundary condition

$$\Phi(\mathbf{x}) \Big|_{\partial\mathcal{V}} = \Phi^0(\mathbf{x}) = \frac{1}{2}\mathbf{Q} \times \mathbf{x} \quad (2.19)$$

—the exact counterpart of (2.3). Indeed, if the volume \mathcal{V} is homogeneous, then $\mathbf{q}(\mathbf{x}) = \frac{1}{2}\nabla \times (\mathbf{Q} \times \mathbf{x}) \equiv \mathbf{Q}$, $\forall \mathbf{x} \in \mathcal{V}$, so that (2.19) corresponds obviously to a constant heat flux \mathbf{Q} throughout \mathcal{V} . Then, in particular, $\bar{\mathbf{q}} \equiv \mathbf{Q}$.

For a heterogeneous RVE, both $\Phi(\mathbf{x})$ and $\mathbf{q}(\mathbf{x})$ fluctuate inside \mathcal{V} . However, the boundary conditions (2.19) yield the validity of (2.15) as if the volume were homogeneous. This fact is a consequence of the statement which is a direct counterpart of Lemma 2.1:

Lemma 2.3 *Whatever the composition and microstructure of the RVE, the volume average of the heat flux is completely determined by the values, $\Phi^0(\mathbf{x})$, of its vector potential $\Phi(\mathbf{x})$ at the boundary $\partial\mathcal{V}$.*

The proof literally repeats the one of Lemma 2.1, having replaced $\nabla\theta(\mathbf{x})$ by $\nabla \times \Phi(\mathbf{x})$. In particular, if the function $\Phi^0(\mathbf{x})$ on $\partial\mathcal{V}$ be the one, given in Eq. (2.19), that corresponds to a constant heat flux in a homogeneous volume \mathcal{V} , then $\bar{\mathbf{q}} = \mathbf{Q}$. Hence, the ‘‘homogeneous’’ boundary condition (2.19) also assures the validity of (2.15), whatever the internal constitution of the medium.

Similarly to the foregoing reasoning, we can solve Eq. (2.13) with the boundary condition (2.19) and find the appropriate mean value of

the temperature gradient $\mathbf{G}^\dagger = \overline{\nabla\theta}$, see Eq. (2.17). The so-obtained \mathbf{G}^\dagger is undoubtedly proportional to the prescribed mean heat flux \mathbf{Q} :

$$\mathbf{G}^\dagger = k^{*\dagger} \mathbf{Q}. \quad (2.20)$$

We *cannot* claim however that the constant $k^{*\dagger}$, as defined in Eq. (2.20), coincides with the effective resistivity k^* , introduced in Eq. (2.17). The reason is that the appropriate temperature gradients $\mathbf{G}^\dagger \neq \mathbf{G}$, since they result from solutions of Eq. (2.13), corresponding to *different* boundary conditions, respectively, to (2.14) and (2.19). The question then arises why (2.14) was preferred when defining the effective resistivity in Eq. (2.17). The answer will be given in Section 1.2.5 below, when discussing the consistency of the definitions of effective conductivity and resistivity, in the sense that they should be each other's inverse. Moreover, it will be shown there (Theorem 2.2) that the homogeneous boundary conditions (2.3) and (2.14) *minimize* the appropriate energies of the RVE as compared to all plausible boundary conditions that give rise to prescribed mean temperature gradient and heat flux respectively. (This will imply in particular that $k^{*\dagger} \geq k^*$.)

1.2.4 Energy Definition of the Effective Constants

Consider the “energy” of the RVE

$$\begin{aligned} \overline{W} &= \overline{W(\mathbf{x}; \nabla\theta(\mathbf{x}))} = \frac{1}{2} \overline{\mathbf{q}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x})}, \\ W(\mathbf{x}; \nabla\theta(\mathbf{x})) &= \frac{1}{2} \kappa(\mathbf{x}) |\nabla\theta(\mathbf{x})|^2. \end{aligned} \quad (2.21)$$

Lemma 2.4 *If the temperature on the boundary $\partial\mathcal{V}$ is $\mathbf{G} \cdot \mathbf{x}$, so that $\overline{\nabla\theta(\mathbf{x})} = \mathbf{G}$, then*

$$\overline{W} = \frac{1}{2} \overline{\mathbf{q}} \cdot \overline{\nabla\theta} = \frac{1}{2} k^* G^2. \quad (2.22)$$

Proof. Let

$$\begin{aligned} \nabla\theta(\mathbf{x}) &= \mathbf{G} + \nabla\theta'(\mathbf{x}), & \mathbf{G} &= \overline{\nabla\theta}, \\ \mathbf{q}(\mathbf{x}) &= \mathbf{Q} + \mathbf{q}'(\mathbf{x}), & \mathbf{Q} &= \overline{\mathbf{q}}, \end{aligned}$$

so that $\nabla\theta'(\mathbf{x})$ and $\mathbf{q}'(\mathbf{x})$ are the fluctuations of the indicated quantities about their mean values \mathbf{G} and \mathbf{Q} respectively. Then

$$\overline{W} = \frac{1}{2} \mathbf{Q} \cdot \mathbf{G} + \frac{1}{2} \overline{\mathbf{q}'(\mathbf{x}) \cdot \nabla\theta'(\mathbf{x})}. \quad (2.23)$$

But

$$\begin{aligned} \overline{\mathbf{q}'(\mathbf{x}) \cdot \nabla \theta'(\mathbf{x})} &= \frac{1}{V} \int_{\mathcal{V}} \mathbf{q}'(\mathbf{x}) \cdot \nabla \theta'(\mathbf{x}) \, d\mathbf{x} \\ &= -\frac{1}{V} \int_{\mathcal{V}} \theta'(\mathbf{x}) \nabla \cdot \mathbf{q}'(\mathbf{x}) \, d\mathbf{x} + \frac{1}{V} \int_{\partial \mathcal{V}} q'_n(\mathbf{x}) \theta'(\mathbf{x}) \, dS = 0, \end{aligned} \quad (2.24)$$

because

$$\nabla \cdot \mathbf{q}'(\mathbf{x}) = \nabla \cdot (\mathbf{q}(\mathbf{x}) - \mathbf{Q}) = \nabla \cdot \mathbf{q}(\mathbf{x}) = 0,$$

and

$$\theta'(\mathbf{x}) \Big|_{\partial \mathcal{V}} = (\theta(\mathbf{x}) - \mathbf{G} \cdot \mathbf{x}) \Big|_{\partial \mathcal{V}} = 0.$$

It follows, in virtue of Eq. (2.23), that

$$\overline{W} = \frac{1}{2} \mathbf{Q} \cdot \mathbf{G} = \frac{1}{2} \kappa^* G^2, \quad (2.25)$$

having used the definition (2.10) of the effective conductivity κ^* of the RVE. \square

It is noted that the above “energy” definition of the effective properties, used in a particular situation already by Einstein [E1a] (see the footnote on page 16), appeared first in Hashin’s papers [HAc] and [HAf] and, independently, in [HIb].

Remark 2.5 *It is important to point out that in the linear case under study, the function $W(\mathbf{x}; \nabla \theta(\mathbf{x}))$ plays the role of a micropotential, i.e.*

$$\mathbf{q}(\mathbf{x}) = \frac{\partial W(\mathbf{x}; \nabla \theta(\mathbf{x}))}{\partial \nabla \theta(\mathbf{x})}$$

in each point $\mathbf{x} \in \mathcal{V}$. Lemma 2.5 then means that

$$\mathbf{Q} = \overline{\mathbf{q}} = \frac{\partial \overline{W}(\mathbf{G})}{\partial \mathbf{G}} = \kappa^* \mathbf{G},$$

so that the average potential $\overline{W}(\mathbf{G}) = \frac{1}{2} \kappa^* G^2$ plays the role of the macropotential. In other words, averaging the micropotential we get just the macropotential; in the latter, the rapidly fluctuating conductivity field $\kappa(\mathbf{x})$ is “smoothed out” being replaced by the effective conductivity κ^* of the RVE.

Consider now the “energy” of the RVE as a function of the dual variable—the heat flux $\mathbf{q}(\mathbf{x})$, i.e.

$$\bar{\Psi} = \frac{1}{2} \overline{\Psi(\mathbf{x}; \mathbf{q}(\mathbf{x}))} = \frac{1}{2} \overline{\mathbf{q}(\mathbf{x}) \cdot \nabla \theta(\mathbf{x})}, \quad (2.26)$$

$$\Psi(\mathbf{x}; \mathbf{q}(\mathbf{x})) = \frac{1}{2} k(\mathbf{x}) |\mathbf{q}(\mathbf{x})|^2.$$

Note that the “energies” W and Ψ , as defined in Eqs. (2.21) and (2.26), coincide, provided the appropriate fields are interconnected by the Fourier law (1.5) and $k(\mathbf{x}) = 1/\kappa(\mathbf{x})$. We shall keep however these different notations for them in order to underline that the “energy” is considered as a functional of different arguments—the temperature and the heat flux fields respectively.

Lemma 2.5 *Let there be no body sources in the RVE. If the heat flux q_n on the boundary $\partial\mathcal{V}$ equals $\mathbf{Q} \cdot \mathbf{n}$, so that $\bar{\mathbf{q}} = \mathbf{Q}$, see Eq. (2.15), then*

$$\bar{\Psi} = \frac{1}{2} \bar{\mathbf{q}} \cdot \nabla \bar{\theta} = \frac{1}{2} k^* Q^2. \quad (2.27)$$

Proof. We repeat the reasoning of the foregoing proof of Lemma 2.4. In the case under study we have again $\overline{\mathbf{q}'(\mathbf{x}) \cdot \nabla \theta'(\mathbf{x})} = 0$, since now $q'_n(\mathbf{x}) = q_n(\mathbf{x}) - \mathbf{Q} \cdot \mathbf{n} = 0$ on $\partial\mathcal{V}$. That is why

$$\bar{\Psi} = \frac{1}{2} \mathbf{Q} \cdot \mathbf{G} = \frac{1}{2} k^* Q^2, \quad (2.28)$$

having used the definition (2.17) of the effective resistivity k^* of the RVE. \square

Remark 2.6 *Similarly to Remark 2.1, it is noted that in the linear case under study the function $\Psi(\mathbf{x}; \mathbf{q}(\mathbf{x})) = \frac{1}{2} k(\mathbf{x}) |\mathbf{q}(\mathbf{x})|^2$ plays the role of a micropotential, i.e.*

$$\nabla \theta(\mathbf{x}) = \frac{\partial \Psi(\mathbf{x}; \mathbf{q}(\mathbf{x}))}{\partial \mathbf{q}(\mathbf{x})}$$

in each point $\mathbf{x} \in \mathcal{V}$. Lemma 2.4 then means that

$$\mathbf{G} = \nabla \bar{\theta} = \frac{\partial \bar{\Psi}(\mathbf{Q})}{\partial \mathbf{Q}} = k^* \mathbf{Q},$$

so that the average potential $\bar{\Psi}(\mathbf{Q}) = \frac{1}{2} k^* Q^2$ plays the role of the macropotential. In other words, averaging the micropotential we get just the macropotential; in the latter the rapidly fluctuating resistivity field $k(\mathbf{x})$ is “smoothed out” and replaced by the effective resistivity k^* of the RVE.

Remark 2.7 Let $\mathbf{q}(\mathbf{x})$ be an arbitrary divergence-free field (not necessarily proportional to $\nabla\theta(\mathbf{x})$). The two Lemmas 2.4 and 2.5 imply that

$$\overline{\mathbf{q}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x})} = \bar{\mathbf{q}} \cdot \nabla\bar{\theta}, \quad (2.29)$$

either for uniform temperature gradient $\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}$ or for uniform flux $q_n(\mathbf{x}) = \mathbf{Q} \cdot \mathbf{n}$ on the boundary $\partial\mathcal{V}$. These two boundary conditions, either of which implies the validity of (2.29), are often called in the literature Hill's.

Note also that Eqs. (2.22) and (2.27) can serve as alternative definitions of the effective conductivity and resistivity, respectively, of the RVE. Their equivalence to the usual definitions (2.10) and (2.17) has several important consequences. One of them will be explored immediately in the next subsection.

1.2.5 Consistency of the Definitions of Effective Properties

The possibility to introduce the effective properties on the base of “energy” notions allows, first of all, a demonstration of the *consistency* for the definitions of the effective conductivity and the effective resistivity, in the sense explained in the following important theorem:

Theorem 2.1 *The effective conductivity and resistivity are each other's inverse, i.e.*

$$k^* = \frac{1}{\kappa^*}. \quad (2.30)$$

Proof. Note first of all that the relations (2.22) and (2.27) do not suffice to claim the validity of Eq. (2.30). The reason is the following. When solving Eq. (2.7) with the boundary condition (2.3), we shall obtain a certain heat flux field $\mathbf{q}(\mathbf{x})$ which is not uniform, in general, on the boundary $\partial\mathcal{V}$, i.e. $q_n(\mathbf{x}) \neq \mathbf{Q} \cdot \mathbf{n}$, where $\mathbf{Q} = \bar{\mathbf{q}}$. The effective resistivity, on the other hand, is defined in Eq. (2.17) under the assumption of homogeneous heat flux on the boundary, see Eq. (2.19). The same remark holds true when considering the solution of the dual BVP (2.13), (2.19)—it generates a temperature field whose temperature gradient does not conform in general with the needed, in the definition (2.10) of the effective conductivity, boundary condition (2.3). That is why the proof of Theorem 2.1 should be preceded by appropriate comparisons between the energies of a

RVE, corresponding to a homogeneous and to a certain inhomogeneous temperature gradients and heat fluxes on the boundary $\partial\mathcal{V}$.⁷

Let first the heat flux be homogeneous on $\partial\mathcal{V}$, i.e. $q_n = \mathbf{Q} \cdot \mathbf{n}$, $\mathbf{x} \in \partial\mathcal{V}$, so that $\bar{\mathbf{q}} = \mathbf{Q}$. The solution of the BVP (2.13), (2.14), generates a temperature field, denoted by $\theta^{(a)}(\mathbf{x})$, whose mean gradient is

$$\mathbf{G} = \overline{\nabla\theta^{(a)}} = k^* \mathbf{Q}.$$

Consider next a second temperature field, $\theta^{(b)}(\mathbf{x})$, corresponding to the uniform temperature gradient $\mathbf{G} \cdot \mathbf{x}$ on the boundary $\partial\mathcal{V}$, i.e. $\theta^{(b)}(\mathbf{x})$ is the solution of the BVP (2.7), (2.3). Obviously, $\overline{\nabla\theta^{(b)}} = \mathbf{G}$, similarly to the field $\theta^{(a)}(\mathbf{x})$. In order to compare the energies, stored by these two fields, consider the difference:

$$\begin{aligned} \overline{W^{(b)}} - \overline{W^{(a)}} &= \overline{W(\mathbf{x}; \nabla\theta^{(b)}(\mathbf{x}))} - \overline{W(\mathbf{x}; \nabla\theta^{(a)}(\mathbf{x}))} \\ &\geq \overline{\left[\nabla\theta^{(b)}(\mathbf{x}) - \nabla\theta^{(a)}(\mathbf{x}) \right] \cdot \frac{\partial W(\mathbf{x}; \nabla\theta^{(a)}(\mathbf{x}))}{\partial \nabla\theta^{(a)}(\mathbf{x})}} \quad (2.31) \\ &= \overline{\left[\nabla\theta^{(b)} - \nabla\theta^{(a)} \right] \cdot \bar{\mathbf{q}}^{(a)}} = 0, \quad \mathbf{q}^{(a)}(\mathbf{x}) = \frac{\partial W(\mathbf{x}; \nabla\theta^{(a)}(\mathbf{x}))}{\partial \nabla\theta^{(a)}(\mathbf{x})}. \end{aligned}$$

Two facts have been used here. The first is Eq. (2.29) which holds since in our case $\mathbf{q}^{(a)}(\mathbf{x})$ corresponds to a uniform heat flux, see Remark 2.7. The second is that the energy function $W(\mathbf{x}; \nabla\theta(\mathbf{x}))$ is convex with respect to $\nabla\theta(\mathbf{x})$ provided $\kappa(\mathbf{x}) > 0$; that is why one of the well-known definitions of convexity is applicable. (Namely, a smooth enough scalar function of a vector argument $f(\mathbf{u})$ is convex, iff $f(\mathbf{v}) - f(\mathbf{u}) \geq (\mathbf{v} - \mathbf{u}) \cdot \nabla f(\mathbf{u})$, $\forall \mathbf{u}, \mathbf{v}$.)

However, in the simplest case under study, when the flux is linearly connected to the temperature gradient, the inequality, used in the second line of Eq. (2.31), can be easily checked, without even referring to convexity arguments. Indeed, in this case it reads

$$\begin{aligned} &\frac{1}{2}\kappa(\mathbf{x}) \left[|\nabla\theta^{(b)}(\mathbf{x})|^2 - |\nabla\theta^{(a)}(\mathbf{x})|^2 \right] \\ &\geq \kappa(\mathbf{x}) \left[\nabla\theta^{(b)}(\mathbf{x}) - \nabla\theta^{(a)}(\mathbf{x}) \right] \cdot \nabla\theta^{(a)}(\mathbf{x}), \end{aligned}$$

⁷In a much more general variational setting this problem has been comprehensively studied by Willis *et al.* [TAc], [TOa], [Wif].

i.e.

$$|\nabla\theta^{(b)}(\mathbf{x})|^2 - |\nabla\theta^{(a)}(\mathbf{x})|^2 \geq 2\nabla\theta^{(a)}(\mathbf{x}) \cdot \nabla\theta^{(b)}(\mathbf{x}) - 2|\nabla\theta^{(a)}(\mathbf{x})|^2,$$

which immediately follows from the obvious inequality

$$\left| \nabla\theta^{(a)}(\mathbf{x}) - \nabla\theta^{(b)}(\mathbf{x}) \right|^2 \geq 0.$$

Thus, Eq. (2.31) implies that $\overline{W^{(b)}} \geq \overline{W^{(a)}}$. But $\overline{W^{(a)}} = \frac{1}{2}k^*Q^2$, according to the definition of the effective resistivity and of the field $\theta^{(a)}(\mathbf{x})$, see Eq. (2.17), while $\overline{W^{(b)}} = \frac{1}{2}\kappa^*G^2$, and therefore

$$\frac{1}{2}\kappa^*G^2 \geq \frac{1}{2}k^*Q^2, \quad \text{i.e.} \quad \kappa^*k^* \geq 1. \quad (2.32)$$

Dually, let $\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}$ on $\partial\mathcal{V}$; through solving the BVP (2.7), (2.3), we find the respective temperature field $\theta(\mathbf{x})$ such that $\overline{\nabla\theta} = \mathbf{G}$; this field generates the heat flux, denoted by $\mathbf{q}^{(a)}(\mathbf{x})$. The mean value of the latter is

$$\mathbf{Q} = \overline{\mathbf{q}^{(a)}} = \kappa^*\mathbf{G}.$$

Consider next a second heat flux field, $\mathbf{q}^{(b)}(\mathbf{x})$, corresponding to the uniform heat flux $\mathbf{Q} \cdot \mathbf{n}$ on the boundary $\partial\mathcal{V}$, i.e. the solution of the BVP (2.13), (2.14). Obviously, $\overline{\mathbf{q}^{(b)}} = \mathbf{Q}$, similarly to the field $\mathbf{q}^{(a)}(\mathbf{x})$. In order to compare the energies, stored by these two fields, consider again the difference:

$$\begin{aligned} \overline{\Psi^{(b)}} - \overline{\Psi^{(a)}} &= \overline{\Psi(\mathbf{x}; \mathbf{q}^{(b)}(\mathbf{x}))} - \overline{\Psi(\mathbf{x}; \mathbf{q}^{(a)}(\mathbf{x}))} \\ &\geq \overline{\left[\mathbf{q}^{(b)}(\mathbf{x}) - \mathbf{q}^{(a)}(\mathbf{x}) \right] \cdot \frac{\partial\Psi(\mathbf{x}; \mathbf{q}^{(a)}(\mathbf{x}))}{\partial\mathbf{q}^{(a)}(\mathbf{x})}} \\ &= \overline{\left[\mathbf{q}^{(b)} - \mathbf{q}^{(a)} \right] \cdot \overline{\nabla\theta^{(a)}}} = 0, \quad \nabla\theta^{(a)}(\mathbf{x}) = \frac{\partial\Psi(\mathbf{x}; \mathbf{q}^{(a)}(\mathbf{x}))}{\partial\mathbf{q}^{(a)}(\mathbf{x})}. \end{aligned} \quad (2.33)$$

We have used, in a manner fully similar to Eq. (2.31), the convexity of the energy function $\Psi(\mathbf{x}; \mathbf{q}(\mathbf{x}))$ with respect to $\mathbf{q}(\mathbf{x})$ (which surely holds if $k(\mathbf{x}) > 0$). Once again Eq. (2.29) was utilized, since in our case $\nabla\theta^{(a)}(\mathbf{x})$ corresponds to a uniform temperature gradient on the boundary, see Remark 2.7. Thus, $\overline{\Psi^{(b)}} \geq \overline{\Psi^{(a)}}$. But $\overline{\Psi^{(a)}} = \frac{1}{2}\kappa^*G^2$, according to the definition of the effective conductivity and of the field $\theta^{(a)}(\mathbf{x})$, see (2.10), while $\overline{\Psi^{(b)}} = \frac{1}{2}k^*Q^2$, and therefore

$$\frac{1}{2}k^*Q^2 \geq \frac{1}{2}\kappa^*G^2, \quad \text{i.e.} \quad \kappa^*k^* \leq 1. \quad (2.34)$$

Comparison of (2.32) and (2.34) proves (2.30). \square

Remark 2.8 *In the multitude of approximate theories of heterogeneous media, a minimum requirement, that each reasonable one should meet, is the consistency of its predictions in the sense of Eq. (2.30). In other words, if we perform the appropriate reasoning, say, for the effective conductivity and for the effective resistivity, the results should be each other's inverse. Without going into details (which are purely technical) we should point out that all the “one-particle” schemes, discussed in Section 1.5 below, are consistent. An explicit check will be performed, for illustrative purposes, only for the self-consistent theory of a polycrystal (see Section 1.6.2). More detailed discussion can be found in [HAh] and [NEa].*

Note that in the proof of the Theorem 2.1 the only fact we have used for the second (“comparison”) fields $\theta^{(b)}(\mathbf{x})$ and $\mathbf{q}^{(b)}(\mathbf{x})$ is that they comply with the conditions (2.4) and (2.15) respectively. That is why, we can claim the validity of the following minimum principles:

Theorem 2.2

(i) *Among all boundary data for the temperature that produce a field $\theta(\mathbf{x})$ with a fixed mean gradient \mathbf{G} , cf. Eq. (2.4), the uniform boundary conditions (2.3) render the “energy” W an absolute minimum W_{\min} ; moreover $W_{\min} = \frac{1}{2}\kappa^*G^2$.*

(ii) *Among all boundary data for a divergence-free (heat flux) field that produce a fixed mean flux \mathbf{Q} , cf. Eq. (2.15), the uniform boundary conditions (2.14) render the “energy” Ψ an absolute minimum Ψ_{\min} ; moreover $\Psi_{\min} = \frac{1}{2}k^*Q^2$.*

These are the two basic minimum principles in the theory of heterogeneous media, based upon the notion of volume averaging. We shall return to them in Section 1.3.4 in connection with the classical variational principles of Dirichlet and Thompson.

Theorems 2.1 and 2.2 clarify the special role of the “homogeneous” boundary conditions (2.3) and (2.14) as well as the reason why they have been adopted when defining the effective conductivity and resistivity. They also explain the reason why a preference was given to to the boundary condition (2.14) when defining the effective conductivity in Eq. (2.17), and not to its “rival” (2.19) (which at first glance looked equally appropriate, generating a homogeneous flux field in a homogeneous medium).

Remark 2.9 Obviously, the central point of the proof of Theorem 2.1 are the inequalities (2.31) and (2.33) which hold for any convex potential W and Ψ . Hence both theorems can be appropriately generalized for mixtures of nonlinearly behaving media, provided the constitutive relations for the constituents emerge from convex potentials (see the book of Nemat-Nasser and Hori [NEa, pp. 47–49] for details and a proof). Here, for the sake of simplicity, the linear scalar case has been only treated. As pointed out by the authors [NEa, pp. 47–48], their proof had been suggested by Willis in a private communication. It is noted also that the above Theorems 2.1 and 2.2 are particular cases of much more general results of Willis et al. [TAc], [TOa], [Wif], which explains why they will be called Willis’.

1.2.6 The “Concentration” Factors

The effective constants can be conveniently represented by means of the so-called “concentration” factors. Determination of these factors, to be defined below, is a problem, equivalent to that of the said constants. However, the appropriate representations provide a natural and useful guide when constructing approximate formulae for the effective properties, as we shall see in Section 1.5.

1.2.6.1 Ideal Thermal Contacts

Let again \mathcal{V} be a RVE of a two-phase medium. Then $\mathcal{V} = \mathcal{V}_1 \cup \mathcal{V}_2$, where \mathcal{V}_1 and \mathcal{V}_2 are the subvolumes, occupied by the constituent ‘ i ’, respectively, $i = 1, 2$.

We shall begin with the scalar conductivity context again. Let us first consider the most common case when an *ideal contact* takes place, so that both temperature and heat flux remain continuous in the whole volume. Then obviously

$$\begin{aligned}\overline{\nabla\theta} &= \phi_1 \langle \nabla\theta \rangle_1 + \phi_2 \langle \nabla\theta \rangle_2, \\ \bar{\mathbf{q}} &= \phi_1 \langle \mathbf{q} \rangle_1 + \phi_2 \langle \mathbf{q} \rangle_2,\end{aligned}\tag{2.35}$$

throughout the volume \mathcal{V} . (If the temperature and heat flux have discontinuities, as it is the case with nonideal contacts, additional terms should be added to the right-hand sides of (2.35), see Eqs. (2.48) and (2.51) below.) In Eq. (2.35)

$$\langle \cdot \rangle_i = \frac{1}{V_i} \int_{\mathcal{V}_i} \cdot \, d\mathbf{x},\tag{2.36}$$

i.e. $\langle \cdot \rangle_i$ signify the spatial averages over the regions \mathcal{V}_i , occupied by the constituent ‘ i ’, $V_i = \text{vol } \mathcal{V}_i$, $i = 1, 2$. According to the Fourier law and the definition of the effective conductivity, see Eq. (2.10),

$$\mathbf{Q} = \bar{\mathbf{q}} = \mathbf{K}^* \cdot \overline{\nabla \theta}, \quad \langle \mathbf{q} \rangle_i = \kappa_i \langle \nabla \theta \rangle_i, \quad i = 1, 2. \quad (2.37)$$

From (2.35) and (2.37) we can exclude the mean temperature gradient in one the phases, say, in ‘1’:

$$\begin{aligned} \mathbf{Q} &= \mathbf{K}^* \cdot \overline{\nabla \theta} = \bar{\mathbf{q}} = \phi_1 \langle \mathbf{q} \rangle_1 + \phi_2 \langle \mathbf{q} \rangle_2 \\ &= \phi_1 \kappa_1 \langle \nabla \theta \rangle_1 + \phi_2 \kappa_2 \langle \nabla \theta \rangle_2 \\ &= \kappa_1 \left(\overline{\nabla \theta} - \phi_2 \langle \nabla \theta \rangle_2 \right) + \phi_2 \kappa_2 \langle \nabla \theta \rangle_2, \end{aligned}$$

or

$$\mathbf{K}^* \cdot \overline{\nabla \theta} = \kappa_1 \overline{\nabla \theta} + \phi_2 [\kappa] \langle \nabla \theta \rangle_2; \quad (2.38)$$

recall that the square brackets denote the appropriate jumps in material properties, e.g. $[\kappa] = \kappa_2 - \kappa_1$, $[\mathbb{L}] = \mathbb{L}_2 - \mathbb{L}_1$, etc.

Let us prescribe, similarly to Section 1.2.2, the average value $\mathbf{G} = \overline{\nabla \theta}$ of the macroscopic gradient, having imposed the boundary condition (2.3) for the temperature. The solution of the boundary value problem (BVP) (2.7), (2.3) depends linearly on the vector \mathbf{G} . Then, in particular,

$$\langle \nabla \theta \rangle_i = \mathbf{A}_i \cdot \mathbf{G}, \quad i = 1, 2, \quad (2.39)$$

with certain *concentration factors* \mathbf{A}_1 and \mathbf{A}_2 that represent, in the case under study, second-rank tensors. (In the scalar and isotropic case the \mathbf{A}_i ’s reduce to constants, called in [REb] *field factors*.)

Note that the concentration factors \mathbf{A}_i are simply interconnected:

$$\phi_1 \mathbf{A}_1 + \phi_2 \mathbf{A}_2 = \mathbf{I}, \quad (2.40)$$

see their definition (2.39) and the first line of Eq. (2.35).

Together with Eq. (2.39) (at $i = 2$), Eq. (2.38) yields the following formula for the effective conductivity tensor of the composite:

$$\mathbf{K}^* = \kappa_1 \mathbf{I} + \phi_2 [\kappa] \mathbf{A}_2, \quad (2.41)$$

or, in an equivalent, but more symmetric form,

$$\phi_1 (\mathbf{K}^* - \kappa_1 \mathbf{I}) \cdot \mathbf{A}_1 + \phi_2 (\mathbf{K}^* - \kappa_2 \mathbf{I}) \cdot \mathbf{A}_2 = 0, \quad (2.42)$$

which follows from Eq. (2.40).

Remark 2.10 *An alternative and physically appealing starting point can be the observation of Landau and Lifshitz [LAa] that the field $\mathbf{q}(\mathbf{x}) - \kappa_1 \nabla \theta(\mathbf{x})$ is non-zero only within the inclusions. That is why its average value,*

$$\overline{\mathbf{q} - \kappa_1 \nabla \theta} = \mathbf{Q} - \kappa_1 \mathbf{G} = [\mathbf{K}^* - \kappa_1 \mathbf{I}] \cdot \mathbf{G},$$

is proportional to the number density n of the inclusions, multiplied by the average value of the same quantity within a “single” inclusion \mathcal{W} :

$$[\mathbf{K}^* - \kappa_1 \mathbf{I}] \cdot \mathbf{G} = \phi_2 \langle \mathbf{q} - \kappa_1 \nabla \theta \rangle_{\mathcal{W}} = \phi_2 [\kappa] \langle \nabla \theta \rangle_{\mathcal{W}}, \quad (2.43)$$

having assumed the inclusions to be of the same shape \mathcal{W} , $\phi_2 = nW$, $W = \text{vol } \mathcal{W}$. Eq. (2.43) obviously reproduces the basic formula (2.41), if (2.39) is taken into account.

Both Eqs. (2.41) and (2.42) look *exceptionally* simple. But this simplicity should not mislead the reader. The extreme difficulties in the homogenization problem, already discussed in Section 1.1, are *not* resolved by Eqs. (2.41) or (2.42); they are only moved from one place to another. That is, instead of looking for the effective conductivity, the quest is now for one of the tensors \mathbf{A}_1 or \mathbf{A}_2 . The specification of any one of them needs knowledge of the temperature fields within the appropriate constituent, say, within *all* of the filler particles. This means that, as a matter of fact, again the detailed solution of the BVP, Eqs. (2.7) and (2.3), is needed. Hence, it is little wonder that the concentration factors can be rigorously determined in a very few cases; moreover, any such case leads to a remarkable formula that gives the effective properties *exactly*, under minimum assumptions about the internal structure of the heterogeneous solids. Two such famous formulae will be discussed in the next Section 1.3. The first one is the Hill expression for the bulk modulus of a two-phase elastic medium, whose constituents possess equal shear moduli, see Eq. (3.66). The other is Levin’s result that interconnects the effective bulk modulus with the effective thermal expansion coefficient, see (3.76).

The formula (2.41) is very convenient, however, for obtaining approximate expressions for the effective properties. The basic idea

is to replace the concentration factor \mathbf{A}_2 in Eq. (2.41) by an appropriate tensor, stemming appropriately from the solution of a single inhomogeneity problem, on the base of certain heuristic arguments. The approximations, devised in such a manner, can be called “one-particle”—they will be discussed in Section 1.5 having, to this end, considered in needed detail the single-inclusion problem in Section 1.4.

Remark 2.11 *The simple and important formula (2.41) is usually attributed to Hill [HIb]. However, in the scalar context it was derived earlier by Reynolds and Hough [REh], who clearly understood and demonstrated its key role in formulating some of the “one-particle” approximations to be treated below.*

1.2.6.2 The Wu Representation

An alternative expression of the effective properties through the concentration factors can be obtained, following a reasoning, sketched by Wu [WUa].

Let $\mathbf{q}(\mathbf{x})$ be the flux in the heterogeneous volume \mathcal{V} , under the “homogeneous” boundary conditions (2.14), and let $\nabla\theta(\mathbf{x}) = k(\mathbf{x})\mathbf{q}(\mathbf{x})$ be the temperature gradient that appears. Consider a “comparison” (or a “reference”) medium with the resistivity k_1 and impose mentally the same flux field $\mathbf{q}(\mathbf{x})$ there; as a result, a certain fictitious “temperature gradient” $\mathbf{g}^c(\mathbf{x})$ will show up:

$$\mathbf{g}^c(\mathbf{x}) = k_1\mathbf{q}(\mathbf{x}) = \begin{cases} \nabla\theta(\mathbf{x}), & \text{if } \mathbf{x} \in \mathcal{V}_1, \\ \frac{k_2}{k_1}\nabla\theta(\mathbf{x}), & \text{if } \mathbf{x} \in \mathcal{V}_2. \end{cases} \quad (2.44)$$

By means of the field $\mathbf{g}^c(\mathbf{x})$, rearrange the energy (2.26) as

$$\begin{aligned} \bar{\Psi} &= \frac{1}{2V} \int_{\mathcal{V}} \mathbf{q}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x}) \, d\mathbf{x} = \frac{1}{2V} \int_{\mathcal{V}} \mathbf{Q} \cdot \mathbf{g}^c(\mathbf{x}) \, d\mathbf{x} \\ &+ \frac{1}{2V} \int_{\mathcal{V}} \left[\mathbf{q}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x}) - \mathbf{Q} \cdot \mathbf{g}^c(\mathbf{x}) \right] \, d\mathbf{x}. \end{aligned} \quad (2.45)$$

The Gauss theorem and the boundary conditions (2.14) yield

$$\int_{\mathcal{V}} \mathbf{q}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x}) \, d\mathbf{x} = \int_{\mathcal{V}} \mathbf{Q} \cdot \nabla\theta(\mathbf{x}) \, d\mathbf{x}.$$

Also

$$\bar{\Psi} = \frac{1}{2}k^*Q^2, \quad \bar{\mathbf{g}}^c = k_1\bar{\mathbf{q}} = \mathbf{Q},$$

see Eqs. (2.26) and (2.44). Hence from (2.45) it follows

$$\begin{aligned} \frac{1}{2}k^*Q^2 &= \frac{1}{2}k_1Q^2 + \frac{1}{2V} \int_{\mathcal{V}} \mathbf{Q} \cdot \mathbf{p}(\mathbf{x}) \, d\mathbf{x}, \\ \mathbf{p}(\mathbf{x}) &= \nabla\theta(\mathbf{x}) - \mathbf{g}^c(\mathbf{x}), \end{aligned} \quad (2.46)$$

where $\mathbf{p}(\mathbf{x})$ is the so-called *polarization field*. Obviously

$$\mathbf{p}(\mathbf{x}) = [\kappa(\mathbf{x}) - \kappa_1] \mathbf{q}(\mathbf{x})$$

which vanishes in the phase ‘1’, see Eq. (2.44). That is why (2.46) can be recast as

$$\frac{1}{2}k^*Q^2 = \frac{1}{2}k_1Q^2 + \frac{1}{2}\phi_2[k] \mathbf{Q} \cdot \langle \mathbf{q} \rangle_2.$$

But

$$\langle \mathbf{q} \rangle_2 = \kappa_2 \langle \nabla\theta \rangle_2, \quad \langle \nabla\theta \rangle_2 = a_2 \mathbf{G},$$

where $\mathbf{A}_2 = a_2 \bar{\mathbf{I}}$ is the concentration factor (2.39) in the isotropic case under study. In turn, $\mathbf{G} = k^* \mathbf{Q}$, and from the last formula the simplest Wu representation emerges:

$$k^* = k_1 + \phi_2[k] k^* \kappa_2 a_2. \quad (2.47)$$

The appropriate generalizations, concerning anisotropic constituents and/or internal alignment, as well as elastic behavior, are obvious. (Wu himself [WUa] considered the elastic case.) However, all the obtained in such a way formulae will be unavoidably equivalent to (2.41): if they are not, by chance, we would have *two* independent relations for the effective tensor and for the concentration factor and they would allow us to specify them both explicitly. The latter is possible but for few simplest cases only such as laminate media, see Remarks 2.1 and 2.2. (The equivalence of Eqs. (2.47) and (2.41) in the isotropic case can be easily checked.)

The above simple considerations possess, however, the merit of invoking the notions of reference media and polarization fields, and that is why they have been included here. The polarization fields are a useful tool in the theory of random heterogeneous media. One of the

reasons is that the basic BVP problems, like (2.7), (2.3) can be easily recast as integral equations with respect to the polarizations. These equations can be then reformulated variationally in an obvious way and in the result the important and very useful variational principles of the so-called Hashin-Shtrikman type emerge, see the survey [Wic] or [WUb].

Simple arguments, employing ingeniously appropriate reference media, can be also utilized to construct the basic approximate schemes of Section 1.5 for the effective properties of heterogeneous media. Details can be found in the paper [BEo].

1.2.6.3 Nonideal Thermal Contacts

In the case of a *nonideal contact* the heat flux and/or the temperature are discontinuous at the interphase boundaries \mathcal{S}_{12} within the volume \mathcal{V} . Accordingly, there are two main types of such contacts—superconducting and resistive, to be properly defined and briefly discussed in Section 1.4.3 below, having introduced the notion of a singular inclusion after Kanaun [KAc]. For the moment it suffices to demonstrate only that the discontinuities of the flux or temperature lead to the appearance of additional terms in Eqs. (2.35).

Indeed, let us start with a “superconducting” interphase, as introduced in Section 1.4.3. Its exact definition is not important here; we need only the fact that the temperature is continuous, but the heat flux has jumps on \mathcal{S}_{12} in this case, see (4.37). Application of Eq. (2.16) then leads to the formula, given recently by Miloh and Benveniste [MIa]

$$\begin{aligned}\bar{\mathbf{q}} &= \frac{1}{V} \int_{\mathcal{V}} \mathbf{q}(\mathbf{x}) \, d\mathbf{x} = \phi_1 \langle \mathbf{q} \rangle_1 + \phi_2 \langle \mathbf{q} \rangle_2 + \bar{\mathbf{q}}^{(12)}, \\ \bar{\mathbf{q}}^{(12)} &= \frac{1}{V} \int_{\mathcal{S}_{12}} [q_n] \mathbf{x} \, dS,\end{aligned}\tag{2.48}$$

where $\mathbf{q}^{(i)}$ is the flux in the phase ‘ i ’, $i = 1, 2$, and \mathbf{n} is the unit normal vector of the interphase surface, pointing from phase ‘2’ to phase ‘1’; hence $[q_n] = \mathbf{q}^{(1)} \cdot \mathbf{n} - \mathbf{q}^{(2)} \cdot \mathbf{n}$ is the jump of the normal component of the flux across \mathcal{S}_{12} . At the same time, the first line of Eq. (2.35) remains unchanged due to continuity of the temperature in the case under study.

Similarly to Eq. (2.39), introduce the *interphase* or *surface concentration factor*, $\mathbf{A}^{(12)}$, through the relation

$$\bar{\mathbf{q}}^{(12)} = \mathbf{A}^{(12)} \cdot \mathbf{G}. \quad (2.49)$$

Repeating literally the elementary reasoning, that led us to (2.41), produces its “superconducting” counterpart

$$\mathbf{K}^* = \kappa_1 \mathbf{I} + \phi_2 [\kappa] \mathbf{A}_2 + \mathbf{A}^{(12)}. \quad (2.50)$$

A fully similar formula can be devised for the the other basic kind of nonideal contact, called “resistance.” Again the exact definition, given in Section 1.4.3 below, is not important in this moment; we need only the fact that the heat flux is continuous in this case (so that the second line of Eq. (2.35) remains now unchanged), but the temperature field has a jump in this case. An application of the Gauss theorem then yields

$$\begin{aligned} \overline{\nabla \theta} &= \frac{1}{V} \int_{\mathcal{V}} \nabla \theta(\mathbf{x}) \, d\mathbf{x} = \phi_1 \langle \nabla \theta \rangle_1 + \phi_2 \langle \nabla \theta \rangle_2 + \bar{\Theta}^{(12)}, \\ \bar{\Theta}^{(12)} &= \frac{1}{V} \int_{S_{12}} (\theta^{(1)} - \theta^{(2)}) \mathbf{n} \, dS, \end{aligned} \quad (2.51)$$

where $\theta^{(i)}$ is the temperature field in the phase ‘ i ’, $i = 1, 2$, and \mathbf{n} is again the unit normal vector on the interphase surface S_{12} , pointing from phase ‘2’ to phase ‘1’, see [BEf] for a detailed derivation and discussion. The counterpart of (2.49) is

$$\bar{\Theta}^{(12)} = \mathbf{B}^{(12)} \cdot \mathbf{G}, \quad (2.52)$$

with $\mathbf{B}^{(12)}$ representing the *interphase concentration factor* for the “resistance” boundary under study. Repeating once again the foregoing reasoning yields now

$$\mathbf{K}^* = \kappa_1 \mathbf{I} + \phi_2 [\kappa] \mathbf{A}_2 - \kappa_1 \mathbf{B}^{(12)}. \quad (2.53)$$

1.2.7 The Elastic Case

The generalization of the foregoing “scalar” reasoning to the elastic case is straightforward, and will be outlined now.

1.2.7.1 The Basic Equations

For a (linear) elastic solid the basic system Eq. (2.7) is replaced by its tensorial counterpart

$$\begin{aligned}\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) &= 0, \\ \boldsymbol{\sigma}(\mathbf{x}) &= \mathbb{L}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}), \quad \boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u} + \mathbf{u} \nabla),\end{aligned}\tag{2.54}$$

so that $\boldsymbol{\varepsilon}(\mathbf{x})$ is the strain tensor, generated by the displacement field $\mathbf{u}(\mathbf{x})$, $\boldsymbol{\sigma}(\mathbf{x})$ is the stress tensor, $\mathbb{L}(\mathbf{x})$ is the fourth-rank tensor of elastic moduli and the colon stands for contraction with respect to two pairs of indices. The analogy with the scalar conductivity case, Eq. (1.5), is obvious: temperature is replaced by displacement, temperature gradient by strain tensor, heat flux by stress tensor, conductivity coefficient $\kappa(\mathbf{x})$ by the elastic moduli tensor $\mathbb{L}(\mathbf{x})$ and the resistivity $k(\mathbf{x}) = 1/\kappa(\mathbf{x})$ by the tensor of elastic compliance $\mathbb{M}(\mathbf{x}) = \mathbb{L}^{-1}(\mathbf{x})$.

All scalar conductivity considerations of Sections 1.2.2 to 1.2.5 are straightforwardly extended to the elastic case. For instance, the counterparts of Lemma 2.1 and its corollary, Eq. (2.6), read:

Lemma 2.6 *Whatever the composition and microstructure of the RVE, the volume average of the strain tensor is completely determined by the displacement field on the boundary $\partial\mathcal{V}$.*

Proof. Let $\mathbf{u}(\mathbf{x})$ be a displacement field in \mathcal{V} , attaining the prescribed boundary values $\mathbf{u}^0(\mathbf{x})$. Using the Gauss theorem, we have

$$\begin{aligned}\bar{\boldsymbol{\varepsilon}} &= \frac{1}{V} \int_{\mathcal{V}} \boldsymbol{\varepsilon}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\mathcal{V}} (\nabla \mathbf{u} + \mathbf{u} \nabla) \, d\mathbf{x} \\ &= \frac{1}{2V} \int_{\partial\mathcal{V}} (\mathbf{n} \mathbf{u}^0 + \mathbf{u}^0 \mathbf{n}) \, dS.\end{aligned}$$

In turn, if $\mathbf{u}^0(\mathbf{x}) = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x} = \mathbf{x} \cdot \boldsymbol{\varepsilon}^0$, where $\boldsymbol{\varepsilon}^0$ is a symmetric tensor of second-rank, then

$$\begin{aligned}\bar{\boldsymbol{\varepsilon}} &= \frac{1}{2V} \int_{\partial\mathcal{V}} (\mathbf{n} \boldsymbol{\varepsilon}^0 \cdot \mathbf{x} + (\boldsymbol{\varepsilon}^0 \cdot \mathbf{x}) \mathbf{n}) \, dS \\ &= \frac{1}{2V} \int_{\mathcal{V}} (\boldsymbol{\varepsilon}^0 \cdot \nabla \mathbf{x} + \boldsymbol{\varepsilon}^0 \cdot (\mathbf{x} \nabla)) \, d\mathbf{x} = \boldsymbol{\varepsilon}^0,\end{aligned}$$

since $\nabla \mathbf{x} = \mathbf{x} \nabla = \mathbf{I}$. \square

Similarly we have

Lemma 2.7 *Whatever the composition and microstructure of RVE, the volume average of the stress tensor, at the absence of body forces, is completely determined by the boundary values of the traction $\mathbf{t}^0 = \boldsymbol{\sigma} \cdot \mathbf{n}$ on $\partial\mathcal{V}$.*

Proof. Let $\boldsymbol{\sigma}(\mathbf{x})$ be a stress field in \mathcal{V} , with the prescribed boundary values of the traction. Due to the assumed absence of body forces, $\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) = 0$ In the Cartesian system x_i , $i = 1, 2, 3$, we have, using the Gauss theorem and the equilibrium equation,

$$\begin{aligned}\bar{\sigma}_{ij} &= \frac{1}{V} \int_{\mathcal{V}} \sigma_{ij}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\mathcal{V}} \delta_{ik} \sigma_{kj}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\mathcal{V}} x_{i,k} \sigma_{kj}(\mathbf{x}) \, d\mathbf{x} \\ &= \frac{1}{V} \int_{\mathcal{V}} (x_i \sigma_{kj}(\mathbf{x}))_{,k} \, d\mathbf{x} - \frac{1}{V} \int_{\mathcal{V}} x_i \sigma_{kj,k}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V} \int_{\partial\mathcal{V}} x_i t_j^0(\mathbf{x}) \, dS,\end{aligned}$$

which indeed is uniquely specified by the traction \mathbf{t}_n^0 on the boundary $\partial\mathcal{V}$.

In turn, if $\mathbf{t}_n^0 = \boldsymbol{\sigma}^0 \cdot \mathbf{n}$ on $\partial\mathcal{V}$, i.e. the traction is uniform on the boundary,

$$\begin{aligned}\bar{\sigma}_{ij} &= \frac{1}{V} \int_{\partial\mathcal{V}} n_p \sigma_{pj}^0 x_i \, dS \\ &= \frac{1}{V} \int_{\mathcal{V}} (\sigma_{pj}^0 x_i)_{,p} \, d\mathbf{x} = \frac{1}{V} \sigma_{pj}^0 \int_{\mathcal{V}} x_{i,p} \delta_{ip} \, d\mathbf{x} = \sigma_{ij}^0,\end{aligned}$$

i.e. $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^0$. \square

1.2.7.2 The Effective Elastic and Compliance Tensors

Similarly to the scalar case, consider first the linear surface displacements

$$\mathbf{u}^0(\mathbf{x}) \Big|_{\partial\mathcal{V}} = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}, \quad (2.55)$$

which assures that $\bar{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}^0$, due to Lemma 2.6.

The BVP (2.54), (2.55) possesses a solution which is unique (the tensor field $\mathbb{L}(\mathbf{x})$ is positive-definite for all $\mathbf{x} \in \mathcal{V}$), which generates a certain stress field $\boldsymbol{\sigma}(\mathbf{x})$. Then

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V} \int_{\mathcal{V}} \mathbb{L}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \, d\mathbf{x} = \mathbb{L}^* : \boldsymbol{\varepsilon}^0. \quad (2.56)$$

The tensor \mathbb{L}^* that enters Eq. (2.56) is the *effective elastic tensor* of the volume \mathcal{V} .

Dually, the stress field $\boldsymbol{\sigma}(\mathbf{x})$ satisfies the equation

$$\nabla \times \boldsymbol{\varepsilon}(\mathbf{x}) \times \nabla = \nabla \times (\mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})) \times \nabla = 0. \quad (2.57)$$

Assume uniform boundary tractions:

$$\mathbf{t}_n^0(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n} \Big|_{\partial\mathcal{V}} = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}, \quad (2.58)$$

which assures that $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^0$, due to Lemma 2.7.

The BVP (2.57), (2.58) possesses a solution which is unique (the compliance tensor $\mathbb{M}(\mathbf{x}) = \mathbb{L}^{-1}(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \mathcal{V}$, once $\mathbb{L}(\mathbf{x})$ is such) which generates a certain strain field $\boldsymbol{\varepsilon}(\mathbf{x})$. Then

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V} \int_{\mathcal{V}} \mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) \, d\mathbf{x} = \mathbb{M}^* : \boldsymbol{\sigma}^0. \quad (2.59)$$

The tensor \mathbb{M}^* that enters Eq. (2.56) is the *effective compliance tensor* of the volume \mathcal{V} .

Let

$$W(\mathbf{x}; \boldsymbol{\varepsilon}(\mathbf{x})) = \frac{1}{2} \boldsymbol{\varepsilon}(\mathbf{x}) : \mathbb{L}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x})$$

be the elastic energy at the point $\mathbf{x} \in \mathcal{V}$. If the linear surface displacements (2.55) are imposed, then

$$\bar{W} = \overline{W(\boldsymbol{\varepsilon}^0)} = \frac{1}{2} \overline{\boldsymbol{\varepsilon}(\mathbf{x}) : \mathbb{L}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x})} = \frac{1}{2} \boldsymbol{\varepsilon}^0 : \mathbb{L}^* : \boldsymbol{\varepsilon}^0. \quad (2.60)$$

Dually, let

$$\Psi(\mathbf{x}; \boldsymbol{\sigma}(\mathbf{x})) = \frac{1}{2} \boldsymbol{\sigma}(\mathbf{x}) : \mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})$$

be the elastic energy at the point $\mathbf{x} \in \mathcal{V}$, considered as a function of the local stresses. If the surface tractions are uniform, see (2.58), then

$$\bar{\Psi} = \overline{\Psi(\boldsymbol{\sigma}^0)} = \frac{1}{2} \overline{\boldsymbol{\sigma}(\mathbf{x}) : \mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})} = \frac{1}{2} \boldsymbol{\sigma}^0 : \mathbb{M}^* : \boldsymbol{\sigma}^0. \quad (2.61)$$

Eqs. (2.60) and (2.61) are the elastic counterparts of the appropriate “scalar” equations (2.22) and (2.27), see Lemmas 2.4 and 2.5. Making use of them, one can show that

$$\mathbb{M}^* = \mathbb{L}^{*-1}, \quad (2.62)$$

i.e. the effective tensors of elasticity and compliance are each other's inverse; the proof repeats almost literally that of the foregoing Theorem 2.1. The minimum properties of the “homogeneous” boundary conditions (2.55) and (2.58) can be then formulated in a manner, fully similar to the statements of Theorem 2.2.

1.2.7.3 The Elastic “Concentration” Factors

In the elastic case only ideal contacts will be treated for which both displacement and normal tractions are continuous at the interphases. In particular, the phases are assumed hereafter firmly bonded, hence no slipping and/or delamination across the interphase boundaries are allowed. The scalar considerations of Section 1.2.7.1 can be then literally repeated, with the only difference that the second-rank concentrations factors \mathbf{A}_i are to be replaced with fourth-rank tensors \mathbb{A}_i such that

$$\langle \boldsymbol{\varepsilon} \rangle_i = \mathbb{A}_i : \boldsymbol{\varepsilon}^0, \quad i = 1, 2. \quad (2.63)$$

These tensors satisfy the identity

$$\phi_1 \mathbb{A}_1 + \phi_2 \mathbb{A}_2 = \mathbb{I},$$

where \mathbb{I} is the “unit” fourth-rank tensor. In Eq. (2.63) $\boldsymbol{\varepsilon}^0$ is the prescribed uniform strain, that stems from the homogeneous boundary condition (2.55).

The effective elastic tensor, for a two-phase medium, now reads

$$\mathbb{L}^* = \mathbb{L}_1 + \phi_2 [\mathbb{L}] : \mathbb{A}_2, \quad (2.64)$$

which is the counterpart of the scalar formula (2.41); \mathbb{L}_i are the tensors of elastic moduli of the constituents, $i = 1, 2$.

Remark 2.12 Recall that any “realistic” tensor of the elastic moduli should possess, besides the symmetry in the first and the second pairs of indices, the “external symmetry”

$$L^{ijkl} = L^{klij}, \quad (2.65)$$

as a consequence of natural thermodynamical requirements. This means that not any fourth-rank tensor can serve as a concentration factor for a heterogeneous medium, even if it satisfies (2.65). The

reason is that the “product” $[\mathbb{L}] : \mathbb{A}_2$ of two tensors with such a symmetry is not obliged to comply with (2.65). Hence, a care is needed when constructing approximate theories, based on the formula (2.64), since they can violate (2.65) for some special internal constitutions (say, certain three-phase media), see Section 1.5.5.2.

Remark 2.13 Nonideal contacts of the same “superconducting” and “resistive” types can be considered in the elastic case as well, extending the reasoning of Section 1.2.6.3. The definition of such contacts due to Kanaun et al. [KA c], [KA d] is outlined below, see Section 1.4.3. An extensive survey of the approaches, results and references, concerning nonideal interphases in elasticity and solid mechanics can be found in the book of Theocharis [TH a], or in [EB a], where the emphasis is more on their material science aspects.

1.2.8 The Effective Absorption Coefficient

Here we shall consider the homogenization quest for Smoluchowski’s absorption problem in a heterogeneous medium (see Section 1.1.3.5).

Formally, it is more convenient and instructive to deal, following Talbot and Willis [TA b], with the more general problem, described by the equation

$$\Delta c(\mathbf{x}) - k^2(\mathbf{x}) c(\mathbf{x}) + K = 0, \quad \mathbf{x} \in \mathcal{V}. \quad (2.66)$$

Additionally, the “no-flux” condition

$$\left. \frac{\partial c(\mathbf{x})}{\partial n} \right|_{\partial \mathcal{V}} = 0 \quad (2.67)$$

is imposed on the boundary $\partial \mathcal{V}$.

The problem (2.66), (2.67) describes, for example, the steady-state diffusion of a species, created at the constant rate K within the volume \mathcal{V} , and absorbed there with variable intensity (defined by the absorption coefficient field $k^2(\mathbf{x})$). For a binary medium, to be only treated here,

$$k^2(\mathbf{x}) = \begin{cases} k_1^2, & \text{if } \mathbf{x} \in \text{constituent '1'}, \\ k_2^2, & \text{if } \mathbf{x} \in \text{constituent '2'}, \end{cases} \quad (2.68)$$

similarly to the conductivity field in Eq. (1.6). Hence the species is absorbed at different rates by the two constituents. Note that

the units are chosen so that in Eq. (2.66) the diffusion coefficient $D = 1$. The condition (2.67) guarantees that the species, created in \mathcal{V} , remains within \mathcal{V} .

A variety of different physical phenomena can be modelled by the system (2.66), (2.67). First, the above mentioned Smoluchowski's problem is recovered if one take the limits:

$$k_1^2 \rightarrow 0, \quad k_2^2 \rightarrow \infty. \quad (2.69)$$

This limit, called by Willis *hard* (due, in particular, to the hard technical difficulties it involves), corresponds obviously to the situation when one of the constituents (the matrix '1') does not absorb at all, while the inclusions (the phase '2') are "perfect" absorbers. This very important case is thoroughly reviewed in Torquato's survey in the present volume (Chapter 2), together with the most recent developments. Boundary conditions more general than (2.67) are discussed there as well.

Note also that the limit (2.69) can be interpreted in terms of heat removal of a solid in the steady-state limit, when a constant heating of intensity K takes place, "competing" with a system of "coolers" (the phase '2') kept at the constant (zero) temperature, see, e.g. [KOa].

In the case of a general binary field $k^2(\mathbf{x})$ an important application of Eq. (2.66) is supplied by the field of irradiation damage: When a solid is subjected to intense, say neutron radiation, defects like vacancies and interstitials are created. They diffuse in the medium and either recombine or are absorbed ("trapped") by the sinks like voids, dislocations or grain boundaries. This leads to a considerable change of the microstructure and, in particular, to swelling of the voids and ultimate rupture. A deep review of this important interpretation and application of Eq. (2.66) can be found in the survey of Brailsford and Bullough [BRa].

To "homogenize" Eq. (2.66) average both sides over the volume \mathcal{V} :

$$\overline{\Delta c(\mathbf{x})} - \overline{k^2(\mathbf{x})c(\mathbf{x})} + K = 0.$$

The Gauss theorem implies

$$\overline{\Delta c(\mathbf{x})} = \frac{1}{V} \int_{\partial\mathcal{V}} \frac{\partial c}{\partial n} dS = 0,$$

due to the no-flux condition (2.67). Hence

$$k^{*2}\bar{c} = \overline{k^2(\mathbf{x})c(\mathbf{x})} = K, \quad \bar{c} = \frac{1}{V} \int_{\mathcal{V}} c(\mathbf{x}) \, d\mathbf{x}, \quad (2.70)$$

which defines the *effective absorption coefficient*, k^{*2} , of the medium.

The sense of Eq. (2.70) is fully similar to that of the definition (2.10) for the effective conductivity. It means, let us underline once again, that from a macroscopic point of view the volume \mathcal{V} looks homogeneous, with a certain effective absorption coefficient k^{*2} . The latter specifies the rate of macroscopical absorption of the species, i.e. the proportionality coefficient (the rate constant) between the mean steady-state concentration \bar{c} and the intensity K of their creation.

Remark 2.14 *It is worth pointing out that a simple change of the sign in the left-hand side of the Helmholtz equation (2.66), with a special form of the source term, drastically changes the physical context. Namely, we recall that the equation*

$$\Delta\Psi(\mathbf{x}) + k_0^2 n^2(\mathbf{x}) \Psi(\mathbf{x}) + \delta(\mathbf{x}) = 0. \quad (2.71)$$

describes the amplitude of a scalar wave, generated by a harmonic point source in the origin, in a lossless, isotropic, time-independent medium. In Eq. (2.71) k_0 is the free-space wave-number and $n(\mathbf{x})$ is the fluctuating index of refraction. The “homogenization” of Eq. (2.71) is an important and classical problem of micromechanics and physics which cannot be discussed here. (The relevant literature is very extensive, see e.g. the survey of Frisch [FRc].) We shall only add that many of the basic ideas and approaches for an approximate evaluation of the effective properties, like self-consistent scheme, effective field, etc., are very well adapted for wave propagation in heterogeneous media and, in particular, for Eq. (2.71), as discussed in detail in Kanaun’s paper in the present volume (Chapter 3). Moreover, a considerable number of them have their direct origin in the study of wave phenomena in such media, as initiated by the works of Foldy [FOa] and Lax [LAd].

Note finally that the rate constant k^{*2} can be expressed by means of the appropriate concentration factors in a manner, fully similar to

the conductivity and elastic cases. Indeed, from (2.70) it follows

$$\begin{aligned}\bar{c} &= \frac{1}{V} \int_{\mathcal{V}} c(\mathbf{x}) \, d\mathbf{x} = \phi_1 \langle c \rangle_1 + \phi_2 \langle c \rangle_2, \\ K &= k^{*2} \bar{c} = \phi_1 k_1^2 \langle c \rangle_1 + \phi_2 \langle c \rangle_2,\end{aligned}\tag{2.72}$$

with the same notations (2.36), cf. Eq. (2.35).

Eliminating $\langle c \rangle_1$ from (2.72) gives

$$k^{*2} \bar{c} = k_1^2 \bar{c} + \phi_2 [k^2] \langle c \rangle_2, \quad [k^2] = k_2^2 - k_1^2.\tag{2.73}$$

This *exact* relation is fully similar to Eq. (2.38). In the present context it defines the effective sink strength k^{*2} through the average concentration $\langle c \rangle_2$ within the inclusions (the phase ‘2’). Hence, if

$$\langle c \rangle_2 = A_2 \bar{c},\tag{2.74}$$

then

$$k^{*2} = k_1^2 + \phi_2 [k^2] A_2,\tag{2.75}$$

which is the “absorption” counterpart of Eqs. (2.41) and (2.64) and, obviously, A_2 is just the concentration factor for the problem under study.

Similarly to the scalar and elastic cases, the formula (2.75) can serve as a convenient starting point when deriving “one-particle” approximations for the effective constant k^{*2} . One of them (the self-consistent one) will be considered in more detail in Section 1.5.7.

1.3 Some Basic Results

In this Section we shall collect several basic results for the effective properties of heterogeneous media. The so-called weakly inhomogeneous medium will be first treated. Though straightforward, its study clarifies why the homogenization problem is so difficult in general: The main reason is that the effective parameters to be specified, though very simple-looking scalar (or tensor) quantities at first glance, incorporate within them *all* details about the internal structure of the medium—a tremendous amount of information, that is.

In practice we however know, as a rule, only a very limited part of the latter. Hence the best we can hope about is, first, to find a certain interval within which the effective parameters should be located (the narrower the better, of course). Such an interval is provided in many cases (but not always, as we shall see) by appropriate variational principles; from them the so-called *variational estimates* for the effective properties result. A brief account will be given below for the classical such estimates, like those of Wiener, Hill, Hashin-Shtrikman and Beran.

Second, with a limited information at hand, we can try to construct certain approximate scheme, using heuristic arguments (like the ones employed by Maxwell, see Section 1.1.3.3, when deriving his famous formula (1.19)). A systematic way of constructing a wide class of such approximate formulae will be discussed in Section 1.5.

1.3.1 Weakly Inhomogeneous Media

The weakly inhomogeneous media consist of phases whose properties do not differ much. For simplicity's sake, we shall additionally assume that they are intermixed in such a manner that the mixture is macroscopically isotropic.

1.3.1.1 The Definition

More precisely, let $\kappa(\mathbf{x})$ be the varying conductivity field of the medium. Represent it in the form

$$\kappa(\mathbf{x}) = \bar{\kappa} + \kappa'(\mathbf{x}), \quad (3.1)$$

where $\kappa'(\mathbf{x})$ is the fluctuation of $\kappa(\mathbf{x})$ about its mean value $\bar{\kappa}$, so that $\overline{\kappa'} = 0$. The medium is *weakly inhomogeneous*, if

$$\max_{\mathbf{x} \in \mathcal{V}} \frac{|\kappa'(\mathbf{x})|}{\bar{\kappa}} \ll 1.$$

For the two-phase materials treated here, the equivalent condition, to be used below, reads

$$|\delta\kappa| \ll 1, \quad \delta\kappa = [\kappa]/\bar{\kappa}. \quad (3.2)$$

It is clear from the definition (3.2) that weakly inhomogeneous media are of very limited practical importance. However, the brief

digression toward their study now is warranted by several facts of primary importance in the general theory, developed in the sequel:

- (i) A simple formula for κ^* , valid to the second-order $(\delta\kappa)^2$ holds; it will play a central role in deriving the famous Hashin-Shtrikman's estimates on κ^* , already applicable for arbitrary two-phase media, see Section 1.3.3 below.
- (ii) The performed analysis will clearly demonstrate that the effective conductivity is indeed a quantity that depends, in general, on *all* details of the internal constitution of a heterogeneous medium.
- (iii) More precisely, it will be seen that macroscopically the internal constitution shows up through certain specific integral parameters that incorporate the so-called correlation functions for the medium.

1.3.1.2 The Perturbation Expansion and the Second-order Approximation

The appearance of the small parameter, $\delta\kappa$, in the BVP (2.7), (2.3), suggests to look, after Brown [BRd], for the solution as the formal perturbation expansion

$$\begin{aligned} \theta(\mathbf{x}) &= \theta^{(0)}(\mathbf{x}) + \theta^{(1)}(\mathbf{x}) + \dots, \quad \theta^{(0)}(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}, \\ \theta^{(p)}(\mathbf{x}) \Big|_{\partial\mathcal{V}} &= 0, \quad \theta^{(p)}(\mathbf{x}) \sim \mathcal{O}((\delta\kappa)^p), \end{aligned} \quad (3.3)$$

$p = 1, 2, \dots$. Then

$$\kappa^* = \bar{\kappa} + \sum_{p=1}^{\infty} B_p, \quad B_p \mathbf{G} = \overline{\kappa'(\mathbf{x}) \nabla \theta^{(p)}(\mathbf{x})}, \quad (3.4)$$

$p = 1, 2, \dots$, as it follows from Eqs. (2.10), (3.1) and (3.3).

The terms of the series (3.3) are specified by means of the equations

$$\bar{\kappa} \Delta \theta^{(1)}(\mathbf{x}) + \mathbf{G} \cdot \nabla \kappa'(\mathbf{x}) = 0, \quad \theta^{(1)}(\mathbf{x}) \Big|_{\partial\mathcal{V}} = 0, \quad (3.5)$$

$$\bar{\kappa} \Delta \theta^{(2)}(\mathbf{x}) + \nabla \cdot (\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})) = 0, \quad \theta^{(2)}(\mathbf{x}) \Big|_{\partial\mathcal{V}} = 0, \quad (3.6)$$

etc., derived in a fully standard way.

Truncation of the series (3.3) after the first term, i.e. taking $\theta(\mathbf{x}) \equiv \mathbf{G} \cdot \mathbf{x}$, results in the already discussed Voigt approximation (2.11).

The simplest nontrivial case shows up, if the series (3.3) is truncated after the second term. Then the perturbation $\theta^{(1)}(\mathbf{x})$ is governed by Eq. (3.5). In turn

$$\bar{\mathbf{q}} = \kappa^* \mathbf{G} = \bar{\kappa} \mathbf{G} + \overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})} + \mathcal{O}((\delta\kappa)^2), \quad (3.7)$$

cf. Eq. (2.10), which means that the performed truncation specifies the effective conductivity κ^* *exactly* to the order $\mathcal{O}((\delta\kappa)^2)$, once the mean value $B_1 \mathbf{G} = \overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})}$ is found.

To find this value, it is noted that the solution of the BVP (3.5) can be written as

$$\theta^{(1)}(\mathbf{x}) = \mathbf{G} \cdot \int_{\mathcal{V}} \nabla_x \frac{\kappa'(\mathbf{y})}{4\pi\bar{\kappa}|\mathbf{x} - \mathbf{y}|} d\mathbf{y}. \quad (3.8)$$

This is clearly an approximation, since the Green function $1/(4\pi|\mathbf{x}|)$ for the Laplace equation in the *unbounded* space is used; in other words, we have tacitly assumed, when solving Eq. (3.5), that the RVE coincides with the whole space \mathcal{R}^3 .

Eq. (3.8) allows us to represent now the quantity, needed in (3.7), in the form

$$\overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})} = \mathbf{G} \cdot \int_{\mathcal{V}} \overline{\kappa'(\mathbf{x}) \kappa'(\mathbf{x} - \mathbf{y})} \nabla_x \nabla_x \frac{1}{4\pi\bar{\kappa}|\mathbf{y}|} d\mathbf{y}. \quad (3.9)$$

The assumptions of statistical homogeneity and isotropy, as discussed in Section 1.2.1, imply in particular that the “two-point” average $\overline{\kappa'(\mathbf{x}) \kappa'(\mathbf{y})}$ depends only on the distance between \mathbf{x} and \mathbf{y} , excepts for a thin layer near the boundary ∂V . To be consistent with usage of the infinite-body Green function, we should neglect this layer, taking in (3.9) the integration domain as the entire \mathcal{R}^3 . Thus

$$\begin{aligned} B_1 \mathbf{G} &= \overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})} \\ &= \mathbf{G} \cdot \int_{\mathcal{R}^3} M_2(r) \nabla \nabla \frac{1}{4\pi\bar{\kappa}r} d\mathbf{x} = -\frac{M_2(0)}{3\bar{\kappa}} \mathbf{G}, \end{aligned} \quad (3.10)$$

since the integral in the last formula represents an isotropic second-rank tensor and $\Delta(1/(4\pi|\mathbf{x}|)) = -\delta(\mathbf{x})$, with $\delta(\mathbf{x})$ denoting the Dirac delta-function. In Eq. (3.10)

$$M_2(r) = \overline{\kappa'(0) \kappa'(\mathbf{z})}, \quad r = |\mathbf{z}|. \quad (3.11)$$

Note that for any “binary” function $a(\mathbf{x})$ that takes the values a_1 and a_2 in the phases \mathcal{V}_1 and \mathcal{V}_2 , respectively, one has

$$\begin{aligned}\overline{a'^2} &= \overline{(a - \bar{a})^2} = \phi_1 \phi_2^2 [a]^2, \\ \overline{a'^3} &= \overline{(a - \bar{a})^3} = \phi_1 \phi_2^2 (\phi_1 - \phi_2) [a]^3,\end{aligned}\tag{3.12}$$

$[a] = a_2 - a_1$, as a simple check demonstrates.

Hence, for the two-phase medium under study,

$$M_2(0) = \overline{\kappa'^2} = \phi_1 \phi_2 [\kappa]^2, \quad B_1 = -\frac{\phi_1 \phi_2 [\kappa]^2}{3\bar{\kappa}}.\tag{3.13}$$

Together with (3.7) and (3.10), this gives the simple, but very important formula,

$$\frac{\kappa^*}{\bar{\kappa}} = 1 - \frac{1}{3} \phi_1 \phi_2 \left(\frac{[\kappa]}{\bar{\kappa}} \right)^2 + \mathcal{O}((\delta\kappa)^2),\tag{3.14}$$

which, in particular, will be needed in Section 1.3.2.4, when deriving the Hashin-Shtrikman’s estimates on the effective conductivity.

To the best of the author’s knowledge, the formula (3.14) was first given by Brown [BRd], and rederived by many authors afterward (especially, see the book [LAA] for an alternative and more heuristic derivation).

Remark 3.1 *The central role of the formula (3.8), and of its consequence (3.14) within the frame of the volume averaging approach, is to be particularly emphasized. From them one can already rigorously derive both Hashin-Shtrikman’s and Beran’s estimates, as we shall see in a moment.*

Remark 3.2 *The “derivation” of (3.10) demonstrates in passing that for a reader with a more rigorous taste, the approach adopted here has profound inherent problems, connected with the employed notion of “very big,” but still finite RVE’s \mathcal{V} (see also the comments of Willis [Wlc, p. 15]). Much more consistent is the stochastic point of view, employed in the pioneering Brown’s paper [BRd], in which the fields like $\kappa(\mathbf{x})$, $\theta(\mathbf{x})$, etc., are treated as random. But this approach, as already pointed out, is not pursued here.*

It is noted that the function $M_2(r)$, defined in Eq. (3.11) is the so-called *two-point correlation* for the medium. The term can be explained by the fact that, while the “one-point” average $\bar{\kappa} = \phi_1\kappa_1 + \phi_2\kappa_2$ provides information about the volume fractions ϕ_i only (at fixed values of κ_i), the “two-point” average $\overline{\kappa'(\mathbf{x})\kappa'(\mathbf{y})}$ supplies already much more detailed “two-point” information, concerning the spatial distribution of the constituents within the heterogeneous medium. It is a simple exercise to show that $M_2(r)$ is directly connected to the average amount of the phase, say, ‘1’, located at the distance r from the origin, provided the same phase is to be found there. In stochastic terms $M_2(r)$ allows evaluation of the probability that if a rod of length r is “thrown” into the medium, both its ends fall within one and the same constituent, see [FRb], [BEi], [TOe] *et al.*

Remark 3.3 *For the integral (3.10) to be convergent, we have tacitly assumed that $M_2(r)$ decays as $r \rightarrow \infty$. The meaning of this assumption is that there is no “long-range order” in the medium; in the language of elementary probability theory the properties of the medium at the points \mathbf{x} and \mathbf{y} and, in particular, the quantities $\kappa(\mathbf{x})$ and $\kappa(\mathbf{y})$, become uncorrelated as the distance between them increases, $r = |\mathbf{x} - \mathbf{y}| \rightarrow \infty$.*

The formula (3.14) shows that to the order $\mathcal{O}((\delta\kappa)^2)$ the effective conductivity of a macro-isotropic medium does not feel specific details of the internal structure. Even the exact form of the two-point correlation function $M_2(r)$ for $r > 0$ is not required. Only the value of the latter at the origin, $M_2(0)$, that is the volume fractions ϕ_i , affects κ^* to this order. To the higher orders however, starting with $\mathcal{O}((\delta\kappa)^3)$, this is already not true.

1.3.1.3 The Third-order Approximation

Indeed, to see this it suffices to look at the equations that govern the higher-order terms in the expansion (3.3). For example, let us truncate (3.3) after the third term. Then

$$\kappa^* \mathbf{G} = \left(\bar{\kappa} - \frac{\overline{\kappa'^2}}{3\bar{\kappa}} + B_2 \right) \mathbf{G}, \quad B_2 \mathbf{G} = \overline{\kappa'(\mathbf{x})\nabla\theta^{(2)}(\mathbf{x})}. \quad (3.15)$$

The function $\theta^{(2)}(\mathbf{x})$ is governed by Eq. (3.6) and it can be easily found, if we decide to employ Eq. (3.8) (replacing again the volume

\mathcal{V} with the entire \mathcal{R}^3). In particular,

$$B_2 = \frac{\overline{\kappa'^3}}{3\overline{\kappa}^2} I_3^\kappa, \quad \overline{\kappa'^3} = \phi_1 \phi_2 (\phi_1 - \phi_2) [\kappa]^3, \quad (3.16)$$

cf. Eq. (3.12), so that

$$\kappa^* = \overline{\kappa} - \frac{\overline{\kappa'^2}}{3\overline{\kappa}} + \frac{\overline{\kappa'^3}}{3\overline{\kappa}^2} I_3^\kappa + \mathcal{O}((\delta\kappa)^3). \quad (3.17)$$

In the last formula

$$I_3^\kappa = \frac{1}{\overline{\kappa'^3}} \iint M_3^\kappa(\mathbf{x}, \mathbf{y}) \nabla \nabla \frac{1}{4\pi|\mathbf{x}|} : \nabla \nabla \frac{1}{4\pi|\mathbf{y}|} d\mathbf{x} d\mathbf{y} \quad (3.18)$$

is a dimensionless parameter that first appeared (in different notation) in Brown's paper [BRd]. (The notation adopted here aims at preserving similarity between the second- and third-order terms in the expansion (3.17), cf. Eq. (3.9) as well.) Also, in Eq. (3.18)

$$M_3^\kappa(\mathbf{x}, \mathbf{y}) = \overline{\kappa'(0)\kappa'(\mathbf{x})\kappa'(\mathbf{y})} \quad (3.19)$$

is the “three-point” counterpart of the function $M_2(r)$, defined in Eq. (3.11). Naturally, $M_3^\kappa(\mathbf{x}, \mathbf{y})$ can be called *three-point correlation*. It supplies more detailed information about the internal structure of the medium, as compared to the volume fraction and the two-point correlation $M_2(r)$. (In probabilistic terms $M_3(\mathbf{x}, \mathbf{y})$ allows evaluation of the probability that if a triangle, two sides of which coincide with the vectors \mathbf{x} and \mathbf{y} , is thrown into the medium, all its vertices fall within one and the same constituent, see [BEi], [TOe] *et al.*)

Note that I_3^κ is a very important characteristic of a two-phase heterogeneous medium: as we shall see, the same quantity will reappear in a certain simple and natural Ritz's type variational procedure for bounding κ^* , proposed by Beran [BEg], see Section 1.3.4.3 below.

Hence, the truncation of the series (3.3) after the third term determines the effective conductivity κ^* exactly to the order $\mathcal{O}((\delta\kappa)^3)$, provided the parameter I_3^κ is found. Its specification, however, needs knowledge not only of the value $M_3(0, 0)$ at the origin, but of the whole function $M_3(\mathbf{x}, \mathbf{y})$ for *all* values of \mathbf{x} and \mathbf{y} (unlike the situation with the function $M_2(r)$ and the corresponding to it second-order term in the expansion (3.3)).

The evaluation of the higher-order terms B_p , $p > 2$, in (3.4) is fully similar: If the validity of Eq. (3.8) is accepted and the RVE is taken unbounded, they can be found in a form, tantamount to (3.17), containing in the integrands the “multi-point averages” (correlation functions) $\overline{\kappa'(\mathbf{x})\kappa'(\mathbf{y}) \cdots \kappa'(\mathbf{w})}$. Explicit formulae and details are supplied by Hori *et al.* [HOa], [HO b]. (In [HO b], [HO c] it is shown that the series (3.3) can be summed under certain additional (and physically reasonable) conditions for the multipoint correlations, corresponding to special kind of heterogeneous media.) The general problem of convergence of the expansions of the type of (3.4) is addressed by Gambin and Kröner [GAa].

The foregoing results show that the effective conductivity κ^* , like any other macroscopical property, depends on the *whole infinite set of all multipoint correlations*, i.e. of the full information about the internal structure of a heterogeneous medium. This very important fact was first demonstrated and clearly stated by Brown [BRd]. The general underlying reason was already pointed out in Section 1.2.1—the nonlinear dependence of the solution of a PDE, like (2.7), upon its coefficients.

As a consequence, any theory that tries to predict the macroscopic properties on the base of limited information is bound to be only an approximation. Hence, a question of central importance for such approximate theories is the existence and the type of realistic heterogeneous media (if any), whose effective properties coincide with those that the theories predict.

1.3.2 The Hashin-Shtrikman Estimates

With a limited information about the internal structure of a medium, the best that one can do is to find an interval, spanned by the plausible effective properties. The more we know, the narrower this interval should be (“collapsing” to the exact value, in principle, if we know “everything,” i.e. the full details of the microstructure). If the medium is two-phase and the volume fractions are solely known, this interval is supplied by the classical Wiener bounds. If we know more—that the medium is also macroscopically isotropic—the Wiener bounds can be narrowed to the Hashin-Shtrikman ones. These basic and fundamental results in the theory of heterogeneous media will be discussed here.

1.3.2.1 The Bergman Formula

For a two-phase heterogeneous solid let us, at the fixed boundary conditions (2.3), change the given conductivity field $\kappa(\mathbf{x})$ to $\kappa(\mathbf{x}) + \delta\kappa(\mathbf{x})$, with a small $\delta\kappa(\mathbf{x})$, as compared to $\kappa(\mathbf{x})$. (Or, in other words, let us vary $\kappa(\mathbf{x})$.) Note that

$$\delta\kappa(\mathbf{x}) = \chi_1(\mathbf{x})\delta\kappa_1 + \chi_2(\mathbf{x})\delta\kappa_2, \quad (3.20)$$

where $\chi_1(\mathbf{x})$ and $\chi_2(\mathbf{x})$ are the characteristic functions of the regions \mathcal{V}_1 and \mathcal{V}_2 , occupied by the constituents ‘1’ and ‘2’ respectively, and $\delta\kappa_1, \delta\kappa_2$ are the variations of their conductivity. As a result, the temperature field will change by $\delta\theta(\mathbf{x})$, and the effective conductivity—by $\delta\kappa^*$. Since both $\theta(\mathbf{x})$ and $\theta(\mathbf{x}) + \delta\theta(\mathbf{x})$ satisfy the same boundary condition (2.3),

$$\delta\theta(\mathbf{x}) \Big|_{\partial\mathcal{V}} = 0, \quad (3.21)$$

which implies, in particular, that $\overline{\nabla\theta} = \overline{\nabla\theta} + \overline{\nabla\delta\theta} = \mathbf{G}$.

According to the energy definition (2.21) of the effective conductivity

$$\begin{aligned} \frac{1}{2}(\kappa^* + \delta\kappa^*)G^2 &= \frac{1}{2}\overline{(\kappa(\mathbf{x}) + \delta\kappa(\mathbf{x}))|\nabla\theta(\mathbf{x}) + \delta\nabla\theta(\mathbf{x})|^2} \\ &= \frac{1}{2}\overline{\kappa(\mathbf{x})|\nabla\theta(\mathbf{x})|^2} + \frac{1}{2}\overline{\delta\kappa(\mathbf{x})|\nabla\theta(\mathbf{x})|^2} \\ &\quad + \overline{\kappa(\mathbf{x})\nabla\theta(\mathbf{x}) \cdot \delta\nabla\theta(\mathbf{x})}, \end{aligned} \quad (3.22)$$

having neglected quantities of higher orders. The first term in the right-hand side of Eq. (3.22) equals $\frac{1}{2}\kappa^*G^2$, see (2.21). Applying the Green formula for the last term there gives

$$\begin{aligned} \overline{\kappa(\mathbf{x})\nabla\theta(\mathbf{x}) \cdot \delta\nabla\theta(\mathbf{x})} &= \frac{1}{V} \int_{\mathcal{V}} \kappa(\mathbf{x})\nabla\theta(\mathbf{x}) \cdot \delta\nabla\theta(\mathbf{x}) \, d\mathbf{x} \\ &= -\frac{1}{V} \int_{\mathcal{V}} \delta\theta(\mathbf{x})\nabla \cdot (\kappa(\mathbf{x})\nabla\theta(\mathbf{x})) \, d\mathbf{x} \\ &\quad + \frac{1}{V} \int_S \kappa(\mathbf{x})\delta\theta(\mathbf{x}) \frac{\partial\theta(\mathbf{x})}{\partial n} \, dS, \end{aligned} \quad (3.23)$$

which vanishes, in virtue of (2.7) and (3.21). Hence

$$\delta\kappa^*G^2 = \overline{\delta\kappa(\mathbf{x})|\nabla\theta(\mathbf{x})|^2} = \overline{\delta\kappa_1\chi_1(\mathbf{x})|\nabla\theta(\mathbf{x})|^2} + \overline{\delta\kappa_2\chi_2(\mathbf{x})|\nabla\theta(\mathbf{x})|^2},$$

which means that

$$\frac{\partial \kappa^*}{\partial \kappa_i} = \frac{1}{G^2} \overline{\chi_i(\mathbf{x}) |\nabla \theta(\mathbf{x})|^2}, \quad i = 1, 2. \quad (3.24)$$

The important formula (3.24) was first noticed (and exploited for bounding the effective properties) by Bergman [BEk], and that is why we shall refer to it as *Bergman's*. In the foregoing reasoning we have followed the more rigorous derivation of Bobeth and Diener [BOa], who rediscovered it later on. One more independent derivation was given recently by Matheron [MAi].

The formula (3.24) has a simple interpretation. Imagine that, for a given two-phase medium, we start varying the properties κ_i of the constituents. As a result, the effective conductivity will become a function of κ_i , i.e. $\kappa^* = \kappa^*(\kappa_1, \kappa_2)$. The formula (3.24) then means that the mean energy, accumulated within each one of the constituents, i.e. $\overline{\chi_i(\mathbf{x}) |\nabla \theta(\mathbf{x})|^2}$, is proportional to the partial derivatives $\partial \kappa^* / \partial \kappa_i$, $i = 1, 2$.

1.3.2.2 The Matheron Inequalities

Since $\chi_i(\mathbf{x})$, as a characteristic function, takes only the values 0 and 1, $\chi_i^2(\mathbf{x}) = \chi_i(\mathbf{x})$. Then

$$\left| \int_{\mathcal{V}} \chi_i(\mathbf{x}) \nabla \theta(\mathbf{x}) \, d\mathbf{x} \right|^2 \leq \int_{\mathcal{V}} \chi_i(\mathbf{x}) \, d\mathbf{x} \int_{\mathcal{V}} \chi_i(\mathbf{x}) |\nabla \theta(\mathbf{x})|^2 \, d\mathbf{x},$$

as it follows from the Schwartz inequality. Obviously

$$\int_{\mathcal{V}} \chi_i(\mathbf{x}) \, d\mathbf{x} = V_i.$$

Recalling that $\phi_i = V_i/V$, we get from (3.24) the inequalities

$$\frac{\partial \kappa^*}{\partial \kappa_i} \geq \frac{1}{\phi_i G^2} \left(\overline{\chi_i(\mathbf{x}) |\nabla \theta(\mathbf{x})|} \right)^2, \quad i = 1, 2, \quad (3.25)$$

pointed out by Matheron [MAi].

Following now the reasoning of the same Matheron's paper [MAi], note that for the two-phase medium under study one has

$$\chi_1(\mathbf{x}) = \frac{\kappa_2 - \kappa(\mathbf{x})}{\kappa_2 - \kappa_1}, \quad \chi_2(\mathbf{x}) = \frac{\kappa(\mathbf{x}) - \kappa_1}{\kappa_2 - \kappa_1}, \quad (3.26)$$

because $\kappa(\mathbf{x})$, as a binary function, takes the values κ_i in the phase ‘ i ’, $i = 1, 2$. Using the definition (2.10) of the effective conductivity together with (3.26) yields

$$\overline{\chi_1(\mathbf{x})\nabla\theta(\mathbf{x})} = \frac{\kappa_2 - \kappa^*}{\kappa_2 - \kappa_1} \mathbf{G}, \quad \overline{\chi_2(\mathbf{x})\nabla\theta(\mathbf{x})} = \frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} \mathbf{G},$$

in virtue of Matheron’s inequalities (3.25). Hence

$$\frac{\partial\kappa^*}{\partial\kappa_1} \geq \frac{1}{\phi_1} \left(\frac{\kappa_2 - \kappa^*}{\kappa_2 - \kappa_1} \right)^2, \quad \frac{\partial\kappa^*}{\partial\kappa_2} \geq \frac{1}{\phi_2} \left(\frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} \right)^2. \quad (3.27)$$

1.3.2.3 The Wiener Bounds

Note next that κ^* is a homogeneous function (of first degree) of κ_1 and κ_2 , i.e. $\kappa^*(\lambda\kappa_1, \lambda\kappa_2) = \lambda\kappa^*(\kappa_1, \kappa_2)$, $\forall\lambda \geq 0$. Then

$$\kappa^* = \kappa_1 \frac{\partial\kappa^*}{\partial\kappa_1} + \kappa_2 \frac{\partial\kappa^*}{\partial\kappa_2} \geq \frac{\kappa_1}{\phi_1} \left(\frac{\kappa_2 - \kappa^*}{\kappa_2 - \kappa_1} \right)^2 + \frac{\kappa_2}{\phi_2} \left(\frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} \right)^2.$$

The latter inequality can be simply factorized to give

$$(\kappa^v - \kappa^*)(\kappa^* - \kappa^r) \geq 0, \quad (3.28)$$

where κ^v and κ^r are the Voigt and Reuss approximations, see (2.11) and (2.18). Since $\kappa^r \leq \kappa^v$ for all $\kappa_i > 0$, $\phi_1 + \phi_2 = 1$, Eq. (3.28) has as a consequence

$$\left(\overline{1/\kappa} \right)^{-1} \leq \kappa^* \leq \bar{k}. \quad (3.29)$$

Hence the Reuss and Voigt values supply an interval within which the effective conductivity of the heterogeneous solid should always lie, *independently* on the details of the internal (macroscopically isotropic) constitution. In the scalar (dielectric, more precisely) context this important fact has been first proved by Wiener [W1a], by means of certain algebraic arguments. That is why the bounds (3.29) are often called *Wiener’s*.

It is important to point out that the bounds (3.29) are *sharp*, in the sense that there exist heterogeneous solids whose conductivity equals the limiting values κ^r and κ^v . (Such solids are the simple laminate or fiber media, already discussed in Remarks 2.1 and 2.2.)

Remark 3.4 Both media whose effective conductivities (along certain directions) coincide with the Voigt and Reuss values are anisotropic. If, additionally, it is required that the medium be macroscopically isotropic, then there exists an interval of admissible values of κ^* , narrower than (3.29). This is one of the most remarkable facts in the theory of heterogeneous media. The narrower interval is specified by the so-called Hashin-Shtrikman's bounds, to be derived in a moment.

1.3.2.4 The Hashin-Shtrikman Bounds

To get more restrictive bounds consider, again after Matheron [MAi], the function

$$F(\kappa_1) = \frac{1}{\kappa_2 - \kappa^*} - \frac{1}{\phi_1(\kappa_2 - \kappa_1)}. \quad (3.30)$$

Here, for the given two-phase medium, the conductivity κ_2 of the phase '2' has been fixed, so that κ^* depends on κ_1 solely. The derivative

$$\frac{dF}{d\kappa_1} = \frac{1}{(\kappa_2 - \kappa^*)^2} \left[\frac{\partial \kappa^*}{\partial \kappa_1} - \frac{1}{\phi_1} \left(\frac{\kappa_2 - \kappa^*}{\kappa_2 - \kappa_1} \right)^2 \right] \geq 0,$$

as a consequence of the first of the inequalities (3.27). Therefore $F(\kappa_1)$ is an increasing function of κ_1 and, consequently, if $\kappa_1 > \kappa_2$,

$$F(\kappa_1) \geq F_0, \quad F_0 = \lim_{\kappa_1 \rightarrow \kappa_2 + 0} F(\kappa_1). \quad (3.31)$$

(If $\kappa_1 < \kappa_2$, the opposite inequality holds.) The evaluation of the limit F_0 is straightforward, using the formula (3.14) and the final result reads

$$F_0 = \frac{B_1}{\phi_1^2 \kappa_2} \quad \text{or} \quad F_0 = -\frac{\phi_2}{3\kappa_2 \phi_1}, \quad (3.32)$$

having recalled the value of B_1 from (3.14).

Remark 3.5 This is the only place in the reasoning, yielding the Hashin-Shtrikman estimates, where the approximation (3.8) and its consequence (3.14) are to be used, together with the value of B_1 from (3.13). If this value is left unspecified, from the considerations below the appropriate HS bounds for a finite body can be derived as well. However, the "finite-body" Green function should be then invoked. As a result the explicit evaluation of B_1 will be extremely difficult even for the simplest regions \mathcal{V} (say a ball), when this function is

known. Moreover, the constant B_1 will then “feel” both the details of the internal structure (through the two-point correlation) and the shape of the RVE, \mathcal{V} .

Inserting F_0 from the second equality of (3.32) in (3.31) gives

$$F(\kappa_1) = \frac{1}{\kappa_2 - \kappa^*} - \frac{1}{\phi_1(\kappa_2 - \kappa_1)} \geq -\frac{\phi_2}{3\kappa_2\phi_1}$$

which can be recast in the more compact form

$$\kappa^* \geq \bar{\kappa} - \frac{\phi_1\phi_2[\kappa]^2}{3\kappa_2 - \phi_2[\kappa]}, \quad \text{if } \kappa_1 > \kappa_2. \quad (3.33)$$

The opposite inequality holds, if $\kappa_1 < \kappa_2$.

In a fully similar manner, the function

$$F(\kappa_2) = \frac{1}{\kappa^* - \kappa_1} - \frac{1}{\phi_2(\kappa_2 - \kappa_1)}$$

can be considered, instead of (3.30), with κ_1 being fixed. Application of the second of the inequalities (3.27) will ensure that $F(\kappa_2)$ is decreasing. Hence, for $\kappa_1 > \kappa_2$, a *lower bound* on κ^* shows up—it has the same form as (3.33), but with indices ‘1’ and ‘2’ interchanged. Hence, together with (3.33), we have

$$\begin{aligned} \kappa_{\text{HS}}^- \leq \kappa^* \leq \kappa_{\text{HS}}^+, \quad \text{if } \kappa_1 > \kappa_2, \\ \kappa_{\text{HS}}^- = \bar{\kappa} - \frac{\phi_1\phi_2[\kappa]^2}{3\kappa_2 - \phi_2[\kappa]}, \quad \kappa_{\text{HS}}^+ = \bar{\kappa} - \frac{\phi_1\phi_2[\kappa]^2}{3\kappa_1 + \phi_1[\kappa]}. \end{aligned} \quad (3.34)$$

For $\kappa_1 < \kappa_2$, the same inequalities (3.34) hold, but with reversed lower and upper values of the bounds.

The bounds (3.34) coincide with the ones derived by Hashin and Shtrikman [HA1] by means of an original variational procedure. A simple check demonstrates that they are more restrictive than the Wiener bounds, given in (3.29).

Note that the upper bound in Eq. (3.34) can be easily recast in a form, coinciding with the Maxwell formula (1.19). This means that, whatever the internal structure of a (macroscopically isotropic) medium, Eq. (1.19) always provides an upper estimate on the effective conductivity, if the matrix is “stiffer” than the inclusions ($\kappa_1 > \kappa_2$) and a lower one in the opposite case ($\kappa_1 < \kappa_2$).

In principle, the generalization of the HS bounds to the elastic case can be obtained in a similar manner, though the technical details will be much more cumbersome. The original derivation, using the Hashin-Shtrikman variational principle [HAK], can be found in the paper [HAM], see also [WId]. For the bulk modulus, however, much simpler derivation can be proposed, following certain Hill's arguments [HIb], as we shall see in Section 1.3.5 below (cf. Eq. (3.68)).

1.3.3 The Hashin Assemblage

The Hashin-Shtrikman (HS) bounds (3.34), apart from their extreme simplicity, possess also the very important properties that they, similarly to the Voigt and Reuss bounds, are *sharp* [HAe]. In other words, they are the narrowest bounds on the effective conductivity that can be constructed, provided we know that the medium is two-phase, macroscopically isotropic, and has prescribed volume fractions ϕ_1, ϕ_2 of the constituents.

For a demonstration that the HS bounds are sharp it suffices to construct special two-phase media whose conductivities coincide with the values κ_{HS}^- and κ_{HS}^+ . These are the so-called *Hashin's assemblages* which look as follows [HAe].

The typical element of the assemblages is a composite sphere, denoted by $\mathcal{V}_{a,b}$. It has an external radius b and contains a concentric spherical inclusion of the radius a , whose conductivity is, say, κ_2 . The coating around the latter, i.e. the region $a < r < b$, has the conductivity κ_1 . If ϕ_2 is the given volume fraction of the phase '2', we require that

$$a^3/b^3 = \phi_2. \quad (3.35)$$

Next we fill up the whole space (the RVE, more precisely), with such composite spheres of different external radius b , from finite down to infinitesimally small. The obtained two-phase medium is just the Hashin assemblage.⁸ The condition (3.35) assures that the volume fractions of the constituents equal the prescribed values ϕ_2 and $\phi_1 = 1 - \phi_2$.

Since the structural elements of the assemblage are fully similar, and differ only in a scale factor, the temperature on their surfaces will be the same, coinciding with the one imposed on the macroscopic

⁸It is noted in passing that the assemblage is an excellent example of a *self-similar* or *fractal-like* structure which looks one and the same in all length scales.

boundary, see Eq. (2.3). Thus, to find the effective conductivity of the composite, it suffices to specify the temperature field within a single composite sphere, i.e. to find the continuous function $\theta(\mathbf{x})$, such that

$$\begin{aligned} \Delta\theta(\mathbf{x}) = 0, \quad \theta(\mathbf{x}) \Big|_{r=b} &= \mathbf{G} \cdot \mathbf{x}, \\ \kappa_2 \frac{\partial\theta}{\partial r} \Big|_{r=a-0} &= \kappa_1 \frac{\partial\theta}{\partial r} \Big|_{r=a+0}. \end{aligned} \quad (3.36)$$

The solution of the problem (3.36) has the form $\theta(\mathbf{x}) = \mathbf{G} \cdot \nabla\varphi(r)$, cf. (1.9), with the potential function

$$\varphi(r) = \begin{cases} \frac{1}{2}C_1r^2, & \text{if } r < a, \\ \frac{1}{2}C_2r^2 - C_3a^3/r, & \text{if } a < r < b. \end{cases} \quad (3.37)$$

The boundary conditions (3.36) elementary specify the unknown constants:

$$C_1 = \frac{(\phi_2 - \phi_1)\beta}{1 - \phi_1\beta}, \quad C_2 = \frac{1}{1 - \phi_1\beta}, \quad C_3 = -\frac{\beta}{1 - \phi_1\beta}, \quad (3.38)$$

with β given in Eq. (1.15).

The mean flux in the RVE coincides with its mean value over the typical composite sphere $\mathcal{V}_{a,b}$:

$$\begin{aligned} \bar{\mathbf{q}} &= \kappa^a \mathbf{G}, \quad \bar{\mathbf{q}} = \langle \mathbf{q} \rangle_{\mathcal{V}_{a,b}}, \\ \langle \mathbf{q} \rangle_{\mathcal{V}_{a,b}} &= \frac{1}{V_{a,b}} \int_{\mathcal{V}_{a,b}} \mathbf{q}(\mathbf{x}) \, d\mathbf{x} = \frac{1}{V_{a,b}} \int_{\mathcal{V}_{a,b}} \kappa(\mathbf{x}) \nabla\theta(\mathbf{x}) \, d\mathbf{x} \\ &= \frac{1}{V_{a,b}} \left[\kappa_2 \int_{r < a} \nabla\theta(\mathbf{x}) \, d\mathbf{x} + \kappa_1 \int_{a < r < b} \nabla\theta(\mathbf{x}) \, d\mathbf{x} \right], \end{aligned} \quad (3.39)$$

where κ^a is the effective conductivity of the assemblage under study.

Elementary calculations, eventually give

$$\kappa^a = \kappa_1 \left(\frac{1 + 2\beta\phi_2}{1 - \beta\phi_2} \right), \quad (3.40)$$

having used that $\theta(\mathbf{x}) = \mathbf{G} \cdot \nabla\varphi(r)$, with $\varphi(r)$ already found in Eqs. (3.37) and (3.38), the isotropy of the integrals that enter Eq. (3.39), as well as the condition (3.35).

Eq. (3.40) obviously coincides with the Maxwell formula (1.19). The latter, as already pointed out, is always one of the HS bounds (3.34). To get the other of the bounds one should only reverse the indices ‘1’ and ‘2’ of the phases (i.e. the phase ‘1’ will be now surrounded by an appropriate concentric layer of ‘2’, such that $a^3/b^3 = \phi_1$, cf. (3.35)). This observation completes the proof that, as far as the scalar conductivity is concerned, the HS bounds (3.34) are indeed optimal for the given amount of information about the medium (macroscopically isotropic two-phase mixtures with prescribed volume fractions).

1.3.4 The Variational Estimates

Consider now the standard variational principles for the transport problems in heterogeneous media, again in the simplest context of scalar conductivity. Their application for bounding the effective properties is a classical one, and will be briefly recalled and summarized. Within the frame of the volume averaging approach, pursued here, they turn out to be of very limited significance, since the boundary values of the admissible fields are prescribed. Instead, the minimum principle of Willis (Theorem 2.2), free of such “boundary” limitations, will to be applied now.

1.3.4.1 The Dirichlet Principle

Let $\theta(\mathbf{x})$ be the *actual* temperature field in a heterogeneous solid, i.e. the solution of Eq. (2.7) with the boundary condition (2.3). Consider the class \mathcal{A} of *admissible* (or trial) fields which are continuous and almost everywhere differentiable, subjected only to the same boundary condition (2.3). Let $\tilde{\theta}(\mathbf{x}) \in \mathcal{A}$, then both $\tilde{\theta}(\mathbf{x})$ and $\theta(\mathbf{x})$ satisfy the same condition (2.3), so that the *variation* $\delta\theta(\mathbf{x})$ should vanish on $\partial\mathcal{V}$:

$$\delta\theta(\mathbf{x}) \Big|_{\partial\mathcal{V}} = 0, \quad \tilde{\theta}(\mathbf{x}) = \theta(\mathbf{x}) + \delta\theta(\mathbf{x}). \quad (3.41)$$

The “energy” of an admissible field, as defined in Eq. (2.21), is a *functional* over the class \mathcal{A} . Its value, for a given field $\tilde{\theta}(\mathbf{x}) \in \mathcal{A}$, is

$$\begin{aligned} \widetilde{W} = \overline{W[\tilde{\theta}(\mathbf{x})]} &= \overline{\frac{1}{2}\kappa(\mathbf{x})|\nabla\tilde{\theta}(\mathbf{x})|^2} = \overline{\frac{1}{2}\kappa(\mathbf{x})|\nabla\theta(\mathbf{x})|^2} \\ &+ \overline{\kappa(\mathbf{x})\nabla\theta(\mathbf{x}) \cdot \delta\nabla\delta\theta(\mathbf{x})} + \overline{\frac{1}{2}\kappa(\mathbf{x})|\nabla\delta\theta(\mathbf{x})|^2}. \end{aligned} \quad (3.42)$$

The middle term in the right-hand side of Eq. (3.42) vanishes, as a consequence of the Gauss theorem, cf. Eq. (3.23). The last term there is non-negative and therefore

$$\overline{W} \leq \widetilde{W}, \quad \overline{W} = \frac{1}{2} \kappa^* G^2, \quad (3.43)$$

having recalled Eq. (2.25) as well. Hence the actual field in the medium *minimizes* the “energy” functional W in the class \mathcal{A} of admissible fields.

The statement (3.43) represents the first of the standard variational principles for the BVP (2.7), (2.3). It is often called *Dirichlet principle* (since, for a homogeneous medium, when $\kappa(\mathbf{x}) = \text{const}$, it states that the solution of the Dirichlet problem $\Delta\theta(\mathbf{x}) = 0$, $\theta(\mathbf{x})|_{\partial\mathcal{V}} = \theta_0(\mathbf{x})$, with a prescribed function $\theta_0(\mathbf{x})$, minimizes the Dirichlet integral $\int_{\mathcal{V}} |\nabla\theta(\mathbf{x})|^2 d\mathbf{x}$).

1.3.4.2 The Thompson Principle

Dually, let $\mathbf{q}(\mathbf{x})$ be the actual heat flux in the medium, i.e. the solution of the BVP (2.13), (2.19). Consider the class \mathcal{B} of *admissible* flux fields $\tilde{\mathbf{q}}(\mathbf{x})$ which are continuous and almost everywhere differentiable, such that

$$\nabla \cdot \tilde{\mathbf{q}}(\mathbf{x}) = 0, \quad \tilde{\mathbf{q}} \cdot \mathbf{n} \Big|_{\partial\mathcal{V}} = \mathbf{Q} \cdot \mathbf{n}. \quad (3.44)$$

Then, the variation $\delta\mathbf{q}(\mathbf{x}) = \tilde{\mathbf{q}}(\mathbf{x}) - \mathbf{q}(\mathbf{x})$ is divergence-free and vanishes on the boundary $\partial\mathcal{V}$:

$$\nabla \cdot \delta\mathbf{q}(\mathbf{x}) = 0, \quad \delta\mathbf{q} \cdot \mathbf{n} \Big|_{\partial\mathcal{V}} = 0. \quad (3.45)$$

The “energy” of an admissible field, as defined in Eq. (2.26), is a *functional* over the class \mathcal{B} . Its value, for an admissible flux field $\tilde{\mathbf{q}}(\mathbf{x}) \in \mathcal{B}$, is

$$\begin{aligned} \tilde{\Psi} = \overline{\Psi[\tilde{\mathbf{q}}(\mathbf{x})]} &= \frac{1}{2} \overline{k(\mathbf{x})|\tilde{\mathbf{q}}(\mathbf{x})|^2} = \frac{1}{2} \overline{k(\mathbf{x})|\tilde{\mathbf{q}}(\mathbf{x})|^2} \\ &+ \overline{k(\mathbf{x})\mathbf{q}(\mathbf{x}) \cdot \delta\mathbf{q}(\mathbf{x})} + \frac{1}{2} \overline{k(\mathbf{x})|\delta\mathbf{q}(\mathbf{x})|^2}. \end{aligned} \quad (3.46)$$

The last term in the right-hand side of Eq. (3.46) is non-negative. The middle term there vanishes, in virtue of Eq. (3.45):

$$\begin{aligned} \overline{k(\mathbf{x})\mathbf{q}(\mathbf{x}) \cdot \delta\mathbf{q}(\mathbf{x})} &= \frac{1}{V} \int_{\mathcal{V}} \nabla\theta(\mathbf{x}) \cdot \delta\nabla\mathbf{q}(\mathbf{x}) d\mathbf{x} \\ &= -\frac{1}{V} \int_{\mathcal{V}} \theta(\mathbf{x}) \nabla \cdot \delta\mathbf{q}(\mathbf{x}) d\mathbf{x} + \frac{1}{V} \int_{\partial\mathcal{V}} \theta(\mathbf{x}) \delta q_n(\mathbf{x}) dS, \end{aligned}$$

having recalled that $\nabla\theta(\mathbf{x}) = k(\mathbf{x})\mathbf{q}(\mathbf{x})$, and employing the Gauss theorem. Therefore,

$$\bar{\Psi} \leq \tilde{\Psi}, \quad \bar{\Psi} = \frac{1}{2}k^*Q^2. \quad (3.47)$$

Hence the actual flux field in the medium *minimizes* the energy functional Ψ in the class \mathcal{B} of admissible fields, defined by means of (3.44).

The statement (3.47) represents the second of the standard variational principles for the heat propagation in a heterogeneous media. Often called *Thompson principle*, it specifies the extremum property of the actual heat flux in such media.

1.3.4.3 The Beran Bounds

The principles (3.43) and (3.47) allow us to derive variational estimates on the effective properties in a standard manner, using appropriate trial fields $\tilde{\theta}(\mathbf{x}) \in \mathcal{A}$ and $\tilde{\mathbf{q}}(\mathbf{x}) \in \mathcal{B}$. Then (3.43) and (3.47) yield

$$\frac{Q^2}{2\tilde{\Psi}} \leq \kappa^* \leq \frac{2\tilde{W}}{G^2}, \quad (3.48)$$

since $k^* = 1/\kappa^*$, see (2.30).

Like many other disciplines, where variational principles are of importance, the art of their applications lies, in general, in the convenient and skillful choice of trial fields. This means that the values of the “energy” can be comparatively easily evaluated for them and the resulting estimates (3.48) should be as close as possible.

As a simplest application of the variational principles (3.43) and (3.47) let us choose as trial fields, respectively, $\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x}$ and $\mathbf{q}(\mathbf{x}) = \mathbf{Q}$. They both are admissible and reproduce the Wiener bounds (3.29), in which only the volume fractions of the constituents show up.

To get more restrictive bounds, broader classes of trial fields should be invoked. For a big, but still finite RVE, a very serious problem immediately arises in this connection, namely, the necessity that the boundary conditions (3.41) and (3.44) be met. Then, if mathematical rigour is to be preserved, the application of the appropriate finite body Green function seems unavoidable, together with a careful limiting passage to an unbounded volume \mathcal{V} . That is why, strictly speaking, the only application of the classical variational principles of

Dirichlet and Thompson here, within the volume averaging approach, is a rederivation of the Wiener bounds. Instead, the Willis minimum principle (Theorem 2.2) should be employed, since it imposes no restrictions on the boundary values of the admissible fields.

To this end, recall the idea of Beran [BEg] to employ as trial fields the truncated perturbation series (3.3), multiplying the terms with adjustable scalars. (This is obviously a Ritz's type variational procedure, with basis functions ingeniously chosen as the terms of the series (3.3).) In the simplest nontrivial case the class

$$\tilde{\theta}(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} + \lambda \theta^{(1)}(\mathbf{x}) \quad (3.49)$$

of trial fields shows up, where $\theta^{(1)}(\mathbf{x})$ is defined in Eq. (3.8), and λ is a certain adjustable constant.

For the trial fields (3.49), the energy (2.21) is a quadratic function of λ

$$\tilde{W} = W[\tilde{\theta}(\mathbf{x})] = \frac{1}{2} (A - 2B\lambda + C\lambda^2) G^2, \quad (3.50)$$

with the coefficients

$$\begin{aligned} A &= \bar{\kappa}, & B &= -\frac{1}{G^2} \mathbf{G} \cdot \overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x})}, \\ C &= \frac{1}{G^2} \left[\bar{\kappa} \overline{|\nabla \theta^{(1)}(\mathbf{x})|^2} + \overline{\kappa'(\mathbf{x}) |\nabla \theta^{(1)}(\mathbf{x})|^2} \right]. \end{aligned} \quad (3.51)$$

The quantity $\overline{|\nabla \theta^{(1)}(\mathbf{x})|^2}$ that appears in the coefficient C can be evaluated, using the equation (3.5) for $\theta^{(1)}(\mathbf{x})$. Indeed, multiply both sides of Eq. (3.5) by $\theta^{(1)}(\mathbf{x})$ and apply the Gauss theorem; the boundary conditions for $\theta^{(1)}(\mathbf{x})$ assure then disappearance of the surface integral, thus yielding

$$\overline{|\nabla \theta^{(1)}(\mathbf{x})|^2} = -\overline{\kappa'(\mathbf{x}) \nabla \theta^{(1)}(\mathbf{x}) \cdot \mathbf{G}} = -B_1 G^2. \quad (3.52)$$

For the second term in the coefficient C , we employ in a similar manner the equations for the functions $\theta^{(1)}(\mathbf{x})$ and $\theta^{(2)}(\mathbf{x})$, see (3.5) and (3.6). The final result is

$$\overline{\kappa'(\mathbf{x}) |\nabla \theta^{(1)}(\mathbf{x})|^2} = \mathbf{G} \cdot \overline{\kappa'(\mathbf{x}) \nabla \theta^{(2)}(\mathbf{x})},$$

and hence

$$C = B_2 - B_1, \quad B = -B_1; \quad (3.53)$$

the second equality is obvious from Eqs. (3.10) and (3.52).

Minimizing the right-hand side of Eq. (3.50) with respect to λ gives the estimate

$$\kappa^* \leq \kappa_{\text{B}}^+, \quad \kappa_{\text{B}}^+ = A - \frac{B^2}{C} = \bar{\kappa} - \frac{B_1^2}{B_2 - B_1}. \quad (3.54)$$

on the effective conductivity. Eq. (3.54) is a consequence, let us point out once again, of the Willis minimum principle. That is why this estimate, as a result, does not need the explicit form of the perturbation coefficients B_1 and B_2 from the series (3.4). It holds therefore for a finite volume \mathcal{V} as well. (But these coefficients will be, in general, “form-dependent,” since the finite-body Green function, corresponding to the RVE, \mathcal{V} , should be exploited in their evaluation; moreover, even in the macro-isotropic case B_1 will depend on the “whole” two-point correlation function.)

For an unbounded RVE, using the approximation (3.8) and, accordingly, the formulae (3.10) and (3.17) for B_1 and B_2 , respectively, the bound (3.54) takes already the explicit (“form-independent,” so to say) form, due to Beran [BEg]:

$$\kappa^* \leq \kappa_{\text{B}}^+, \quad \kappa_{\text{B}}^+ = \bar{\kappa} \left\{ 1 - \frac{\frac{1}{3} \overline{\kappa'^2}}{\overline{\kappa^2}} \bigg/ \left(1 + \frac{\overline{\kappa'^3}}{\bar{\kappa} \overline{\kappa'^2}} I_3^\kappa \right) \right\}. \quad (3.55)$$

In a fully similar manner the lower Beran bound can be deduced, using the Willis principle. The final result, skipping the purely technical details, reads

$$\kappa_{\text{B}}^- \leq \kappa^*, \quad \kappa_{\text{B}}^- = \kappa^r \left\{ 1 - \frac{\frac{2}{3} \overline{k'^2}}{\overline{k^2}} \bigg/ \left(1 + \frac{1}{2} \frac{\overline{k'^3}}{\bar{k} \overline{k'^2}} (1 + I_3^k) \right) \right\}^{-1}, \quad (3.56)$$

where $\kappa^r = (\overline{1/\kappa})^{-1}$ is the Reuss approximation (2.18) and $k(\mathbf{x}) = 1/\kappa(\mathbf{x})$ is the resistivity field for the medium. The parameter I_3^k has exactly the same form as I_3^κ in Eq. (3.18), but with $\kappa(\mathbf{x})$ replaced by $k(\mathbf{x})$.

For a two-phase medium it is easy to show that $I_3^\kappa = I_3^k$, i.e. the upper and lower Beran bounds depend on a single parameter I_3^k . The latter reflects in a certain integral way the internal structure of the medium, by means of the three-point correlation function $M_3^\kappa(\mathbf{x}, \mathbf{y})$, see (3.19). In this sense the Beran bounds are *three-point* bounds.

It is noted that the foregoing derivation of the Hashin-Shtrikman bounds (3.34) implies that they are *two-point* because only the two-point correlation $M_2(r)$ is needed for their evaluation. (This is the assumption of macro-isotropy that, happily, has left only the value $M_2(0)$ of the latter in the final result.)

Moreover, for a weakly inhomogeneous medium the Beran bounds, κ_{B}^- and κ_{B}^+ coincide with the exact value of the effective conductivity, as given in Eq. (3.17), to the order $\mathcal{O}((\delta\kappa)^3)$. This means that

$$\kappa^* \approx \kappa_{\text{B}}^+ \approx \kappa_{\text{B}}^- = \bar{\kappa} - \frac{\overline{\kappa^2}}{3\bar{\kappa}} + \frac{\overline{\kappa^3}}{3\bar{\kappa}^2} I_3^\kappa + \mathcal{O}((\delta\kappa)^3). \quad (3.57)$$

The sign \approx indicates here that the appropriate quantities differ in the order $\mathcal{O}((\delta\kappa)^3)$. In this sense the Beran bounds are *third-order* ones.

The formula (3.57) well illustrates a basic and well-known feature of variational estimates (that holds not only in the context of heterogeneous media). Namely, the more structural information is incorporated, the narrower the bounds become. Indeed, for the simplest Wiener's bounds (3.29), when the volume fractions are only known in a binary medium

$$\kappa^v - \kappa^r = \phi_1\phi_2[\kappa]^2/\tilde{\kappa},$$

where $\tilde{\kappa}$ is defined in (3.62) below. Hence κ^v and κ^r coincide to the order $\mathcal{O}(\delta\kappa)$; they are therefore *first-order*. The HS bounds (3.34) incorporate the additional information that the medium is statistically isotropic. Accordingly

$$\kappa_{\text{HS}}^+ - \kappa_{\text{HS}}^- = \frac{2\phi_1\phi_2[\kappa]^3}{(2\kappa_1 + \bar{\kappa})(2\kappa_1 + \tilde{\kappa})},$$

so that the coincidence is to the order $\mathcal{O}((\delta\kappa)^2)$; they are therefore *second-order*. Finally, incorporating some (but not full) “three-point” information in the Beran bounds (3.55), (3.56) makes them third-order, as already pointed out.

To conclude the story about Beran's bounds, let us return to the series (3.4). It is obviously the Taylor expansion of the effective conductivity κ^* treated as a function of the parameter $\delta\kappa = [\kappa]/\bar{\kappa}$, see Eq. (3.2). (That is, with the geometry of the two-phase medium being *fixed*, we vary the conductivity of one of the constituents, say

κ_2 , having fixed κ_1 .) This parameter need not be small, in general, for the series to converge. Moreover, it is not even necessary to assume it real—the conductivities can well be complex numbers which, physically, may account for the possible dielectric losses in the medium. Then (3.4) defines a function in the complex plane, which possesses a number of important and beautiful properties. Such a complex-analytical viewpoint was introduced by Bergman [BEk], [BEl], who, having recognized these properties, employed them for deriving bounds on the effective conductivity that hold both in real and complex cases, see also Milton’s papers [MIc], [MIId]. The reasoning of Bergman and Milton was put on a rigorous base by Golden and Papanicolaou [GOa]—they proved that the function $\kappa^* = \kappa^*(\delta\kappa)$ in the complex region can be represented as a certain Stieltjes integral. This representation opened the way for systematic derivation of bounds on κ^* , using truncation of the Taylor series and the so-called Padé approximants, whose definition and a simple application will be very briefly discussed below. Any details of this beautiful theory are beyond the scope of the present elementary survey (see, e.g. [MIh] for a very clear summary of the basic ideas). But, we have accumulated until now some basic results, happily, that will suffice for a small illustration.

Let us truncate the Taylor series (in the point $z = 0$) of a function $f(z)$ after the z^{p+q+1} -term. The rational function $P(z)/Q(z)$ is called (p, q) -Padé approximant for $f(z)$, if its Taylor expansions coincides to the order z^{p+q+1} with the said truncation; here $P(z)$ and $Q(z)$ are polynomials of degrees p and q , respectively, and $Q(0) = 1$. (The origin, importance, theory and numerous applications of such approximations are clarified and collected, e.g. in the book [BAa].)

To apply a Padé’s approximant in the study of effective conductivity κ^* , observe that we already know the Taylor expansion (3.4) of the latter, treated as a function of $\delta\kappa$, to the order $\mathcal{O}((\delta\kappa)^3)$, cf. Eq. (3.57). The simplest nontrivial approximant will be then of the order (1,2) and it should have the form

$$\kappa^* = \bar{\kappa} + (\delta\kappa)^2 \frac{a_0}{1 + b_1 \delta\kappa}, \quad (3.58)$$

as it follows from (3.14). The coefficients a_0 and b_1 are specified by the condition that the Taylor expansion of the function (3.58) coincides to the order $\mathcal{O}((\delta\kappa)^3)$ with that in (3.57). The result, as

immediately seen, reproduces the Beran bound (3.55). Hence, this bound is nothing but a simplest Padé approximant for the function $\kappa^* = \kappa^*(\delta\kappa)$.

Remark 3.6 *In a purely formal manner, consider $\kappa^* = \kappa^*(\phi_2)$ as a function of the volume fraction ϕ_2 of one of the constituents.⁹ For a dispersion of spheres the Taylor expansion of this function is known to the order ϕ_2 , due to Maxwell, see (1.20). We can try to approximate $\kappa^*(\phi_2)$ by a simple Padé's like function:*

$$\kappa^*(\phi_2) \approx \kappa_1 \frac{1 + a_1\phi_2}{1 + b_1\phi_2}. \quad (3.59)$$

To fix the constants in (3.59), we require that it coincides with (1.20) to the order ϕ_2 and has the value κ_2 , if $\phi_2 = 1$. A simple check shows that the right-hand side of Eq. (3.59) reproduces then the Maxwell (1.19) or which is the same, one of the Hashin-Shtrikman bounds (3.34). The author cannot provide any explanation of this fact which could be only a fortunate coincidence. At first glance it is strange as well that starting with the formula (1.20), valid for spherical shape of the inclusions in a dispersion, one gets the HS-bound out of the approximation (3.59), already valid for arbitrary (macro-isotropic) internal geometry.

1.3.4.4 The Torquato-Milton Parameter

The Beran bounds have been considerably simplified by Torquato [TOB] and Milton [MIL]. They introduced the so-called ζ -parameter which, in term of the above defined parameter I_3^κ , can be defined through the relation:

$$3(\phi_2 - \phi_1)I_3^\kappa = 2\zeta_1 + 3\phi_1 - \phi_2, \quad \zeta_2 = 1 - \zeta_1. \quad (3.60)$$

⁹The function $\kappa^* = \kappa^*(\phi_2)$ is very often considered and approximated in the literature on composite media, together with its expansions in powers of ϕ_2 (called *virial*, borrowing the terminology from the theory of dense gases); see Section 1.5 below. Despite this, the reader should be warned that it has in general no exact meaning, if the internal structure is not carefully predefined. The point is that for a given volume fraction ϕ_2 there exist (infinitely) many internal constitutions; changing ϕ_2 by an infinitesimal amount only, this constitution can be drastically changed and rearranged.

By means of ζ 's, the Beran bounds (3.55) and (3.56) adopt the amazingly simple and symmetric form:

$$\left\{ \bar{k} - \frac{2\overline{k'^2}}{2\langle \tilde{k} \rangle + \langle k \rangle_\zeta} \right\}^{-1} \leq \kappa^* \leq \bar{\kappa} - \frac{\overline{\kappa'^2}}{\langle \tilde{\kappa} \rangle + 2\langle \kappa \rangle_\zeta}, \quad (3.61)$$

with the notations

$$\langle \tilde{k} \rangle = \phi_1 k_2 + \phi_2 k_1, \quad \langle k \rangle_\zeta = \zeta_1 k_1 + \zeta_2 k_2, \quad (3.62)$$

and similarly for any other quantity instead of k , see [M1c].

The bounds (3.61) should be more restrictive than the elementary Wiener's bounds (since the appropriate functionals are minimized over broader classes of trial fields). This implies that the denominators in the both fractions in (3.61) should be non-negative, *whatever* the properties of the constituents $\kappa_1, \kappa_2 \geq 0$, which immediately yields

$$0 \leq \zeta_1, \zeta_2 \leq 1. \quad (3.63)$$

The limiting values ζ_1 or $\zeta_2 = 0, 1$ reproduce one of the HS-bounds (3.34). Together with (3.63), this fact implies that the Beran bounds are always *more restrictive* than the Hashin-Shtrikman's ones (something which becomes clear only after the simplification (3.61) of the former). This sounds natural, but by no means is obvious (since the Beran bounds make use of the three-point information *only partially*, and this does not suffice to claim in general that they are better than any two-point ones, like Hashin-Shtrikman's).

The evaluation of the ζ -parameter is a nontrivial and complicated task for a given heterogeneous medium; the formula (3.18) for I_3^κ and the definition (3.60) imply that ζ represents in general a six-fold integral with a singular kernel. The latter should be first drastically simplified before trying to apply numerical or analytical methods.

Considerable efforts have been dedicated to this end, starting perhaps with the series of Corson's papers, see [COa] and the ensuing pages of the same issue of *J. Appl. Phys.* There the needed parameter (ζ as a matter of fact) has been evaluated numerically using the outcome of extensive experimental work, concerned with measurement of two- and three-point correlations of a real two-phase alloy (based on a Buffon's kind of "needle" and "triangle" games).

For special (and perhaps idealized) models of heterogeneous media the parameter ζ was analytically found. For example, one of the first and simplest models due to Miller [MIb], can be recalled here. This is the so-called *cell material*, constructed through dividing the space \mathcal{R}^3 into cells. Each cell is supplied afterward with conductivity κ_1 and κ_2 with probability ϕ_1 and ϕ_2 , respectively, *independently* of the properties of the surrounding cells. For this model both the two- and three-point correlations are quite simple and it turns out, for example, that $\zeta_1 = \phi_1$, in the case of spherical cells, see [MIb], [HOa] *et al.* For other, more realistic and complicated models of heterogeneous media, details and extensive references, concerning the evaluation of the ζ -parameter, are given in Torquato's survey [TOc], see also the recent paper of Jeulin [JEC].

1.3.5 The Bounds in the Elastic Case

All “scalar” considerations, performed until now, can be generalized to the elastic case in an obvious manner. The derivation of the appropriate expansions like (3.17) will be considerably more tedious, due to the tensorial nature of the basic quantities (strain and stress tensors).

There is however another, more important, complication for an elastic heterogeneous solid, namely, the fact that there exist at least *two* small parameters, say, δk and $\delta\mu$ in the isotropic case, instead of the single parameter (3.2) of the scalar case. Both these parameters will be small for a weakly inhomogeneous solid, $\delta k, \delta\mu \ll 1$, but they may be small of different orders. Details can be found, e.g., in the papers [MOa] and [LOa]. One of the central “perturbation” results of these works is Eq. (3.67) below. It is however a simple particular case of the general formula of Hill, see (3.66).

The Hashin-Shtrikman's bounds (3.34) can be generalized to the elastic case extending the arguments of Section 1.3.2, once the perturbation expansions of the moduli (to the second order of δk and $\delta\mu$) are known. The original derivation of these bounds employs the appropriate variational principle [HA1], [HAM], see also [WId]. It will be omitted here, due to the number of technical details it employs. Instead only the bound on the effective bulk modulus will be derived below in a different (non-variational) way, following Hill [HIb].

The classical variational principles, based on minimization of the energy of a RVE, \mathcal{V} , are formulated in a straightforward manner for

an elastic medium. Following Hill [HIa] (who dealt with polycrystals, to be precise), the simplest trial fields of homogeneous strain and stress within the volume \mathcal{V} produce the counterpart of the Wiener's bounds (3.29), namely:

$$\begin{aligned} \mathbb{L}^r &\leq \mathbb{L}^* \leq \mathbb{L}^v, \\ \mathbb{L}^v &= \overline{\mathbb{L}(\mathbf{x})}, \quad \mathbb{L}^r = (\overline{\mathbb{L}^{-1}})^{-1}, \end{aligned} \quad (3.64)$$

where \mathbb{L}^v and \mathbb{L}^r are the *Voigt* and *Reuss approximations* for the tensors of the effective moduli, respectively. That is why the bounds (3.64) are often called *Hill's*. For elastic (two-phase) composites their derivation is due also to Paul [PAc], so that sometimes they are referred to as Paul's bounds as well.

The generalization of the Beran's bounds to the elastic case is, in principle, straightforward, though again considerably more cumbersome. For the effective bulk modulus k^* , when the applied macrostrain is spherical, the appropriate bounds are due to Beran and Molyneux [BEj]. They contain the same statistical parameter ζ , that appeared in the scalar bounds (3.61), but this became clear only when Milton [MIc] drastically simplified the original Beran-Molyneux estimates, recasting them as

$$\left\{ \overline{1/k} - \frac{\overline{4(1/k)^{\prime 2}}}{4\langle 1/k \rangle + 3\langle 1/\mu \rangle_{\zeta}} \right\}^{-1} \leq k^* \leq \bar{k} - \frac{3\overline{k^{\prime 2}}}{3\langle \bar{k} \rangle + 4\langle \mu \rangle_{\zeta}} \quad (3.65)$$

Obviously, (3.65) resembles very closely (3.61). (It is recalled that for *any* binary quantity that takes the values, say, a_1 and a_2 in the constituents, $a^{\prime 2} = \overline{(a - \bar{a})^2} = \phi_1\phi_2(a_1 - a_2)^2$, cf. (3.13).)

Remark 3.7 *We shall call Hill's medium an elastic binary mixture of isotropic constituents with the same shear moduli, $\mu_1 = \mu_2 = \mu$, which is macroscopically isotropic. For such a medium $\langle \mu \rangle_{\zeta} = \mu$, $\langle 1/\mu \rangle_{\zeta} = 1/\mu$ so that the parameter ζ disappears from the bounds (3.65). Moreover, a simple check shows that the bounds coincide, yielding the exact value of the effective bulk modulus*

$$k^* = \bar{k} - \frac{\overline{k^{\prime 2}}}{\bar{k} + \frac{4}{3}\mu + \overline{k^{\prime 3}/k^{\prime 2}}}. \quad (3.66)$$

This is a remarkable result due to the fact that it holds independently on the internal structure of the medium, under the only assumptions of macroscopical isotropy and equal shear moduli.

The formula (3.66) is due to Hill [HIb]. His original reasoning, which does not make use of any variational arguments, is based on an ingenious guess for the real displacement field in the medium. This field turns out to be a linear combination of a pure dilatation and of the gravitational force generated by uniform distribution of mass within one of the constituents; the dilatation it generates is piece-wise constant.¹⁰

Remark 3.8 In the weakly inhomogeneous Hill's medium ($\mu_1 = \mu_2$) the perturbation expansion of the type (3.14) reads

$$k^* = \bar{k} - \frac{\overline{k'^2}}{\bar{k} + \frac{4}{3}\mu} + \mathcal{O}((\delta k)^2), \quad \delta k = \frac{[k]}{\bar{k}}, \quad (3.67)$$

and it immediately follows from the general formula (3.66). Moreover Eq. (3.66) specifies easily the perturbation expansion to any order of δk . The particular case (3.67) was found independently in [MOa], [LOa] directly, though the needed calculations are quite tedious.

For the effective shear modulus μ^* the evaluation of the Beran type bounds is due to McCoy [MCa] and it is much more involved than the ones for the conductivity and bulk modulus. Moreover, the bounds include a second statistical parameter of the kind of ζ (the so-called η -parameter of Torquato and Milton, which shows up as a consequence of the tensorial structure of the Green function in the elastic case). A much simpler form, similar to (3.61) and (3.65), of the McCoy bounds on μ^* can be found again in [MIc].

It is to be noted finally in this subsection that the Hill formula (3.66) allows to obtain easily the Hashin-Shtrikman bounds on the bulk modulus of a binary mixture. Indeed, following Hill [HIb], con-

¹⁰Strictly speaking, the Hill analysis only proves that the right-hand side of Eq. (3.66) is an upper bound on k^* . The reason is that the displacement field, devised by him, *does not* satisfy the homogeneous boundary condition (2.55) exactly, and hence this can be only one of the trial displacement fields in the minimum principle of Willis (Theorem 2.2). The mean dilatation is prescribed, but *nothing* is known about the exact values of the displacement on the boundary $\partial\mathcal{V}$.

sider a more general case of an elastic mixture, when $\mu_2 < \mu_1$ and $k_2 < k_1$. (Note that this is a particular case of the so-called “well-ordered” mixture, when $(\mu_2 - \mu_1)(k_2 - k_1) > 0$; the “badly-ordered” one corresponds to the inequality $(\mu_2 - \mu_1)(k_2 - k_1) < 0$.) Keeping the modulus k_1 fixed, let us start increasing mentally μ_2 until it coincides with μ_1 . In this process the effective bulk modulus will increase as well and its value will be the one, given in Eq. (3.66) when μ_2 “reaches” μ_1 . Hence (3.66) will provide an upper bound on k^* in the case under study. In a similar way we can decrease μ_1 until it coincides with μ_2 ; then (3.66) will give a lower bound on k^* , i.e.

$$\bar{k} - \frac{\overline{k'^2}}{\bar{k} + \frac{4}{3}\mu_2 + \overline{k'^3/k'^2}} \leq k^* \leq \bar{k} - \frac{\overline{k'^2}}{\bar{k} + \frac{4}{3}\mu_1 + \overline{k'^3/k'^2}}. \quad (3.68)$$

If $\mu_2 > \mu_1$ and $k_2 > k_1$, the inequality signs are to be changed in (3.68). The same inequalities (3.68) were derived by Hashin and Shtrikman [HAM] by means of variational arguments; these authors, however, were able to find estimates of a similar kind for the effective shear modulus as well.

1.3.6 Cross-Properties Relations: The Levin Formula

Consider again a two-phase medium. Geometrically, this is simply a division (in general, extremely complicated of course) of a region \mathcal{V} into two parts, \mathcal{V}_1 and \mathcal{V}_2 , that represent the subregions occupied by the phases, $\mathcal{V} = \mathcal{V}_1 \cup \mathcal{V}_2$. Such a division, purely geometrical in this moment, can be *materialized* in many different ways and contexts, in the sense that we can fill up the phases with materials of different conductivities, elasticity constants, absorption abilities, etc. We can as well let a fluid penetrate the volume through one of the phases, assuming the other to be a rigid or deformable skeleton and so on and so forth. In any of the cases, pursuing the appropriate homogenization problem, we can evaluate, in principle, the specific effective properties. The fact that behind any one of these problems, a fixed and *common for all of them* geometrical “structure” is hidden (the given division of the volume \mathcal{V} into two subregions \mathcal{V}_1 and \mathcal{V}_2) suggests that the effective properties, no matter how different in context and interpretation, should be interconnected. Such interconnections are often called *cross-properties* relations.

The simplest cross-properties relations appear due to an obvious mathematical analogy between the equations that govern different

phenomena. The already mentioned examples of dielectric permeability, magnetic permittivity, diffusion, heat conduction, etc., provide such examples of full formal analogy; that is why it suffices to get results for one of these phenomena, for the rest only the interpretation should be changed. An analogy of this kind will be used in Section 1.5.2, when deriving the Einstein formula (1.21) from a study of an elastic dispersion of spheres. In some cases, however, the mathematical analogy, though present, is not that obvious and some efforts are needed to clarify it. An example is provided by the heat propagation in a fiber-reinforced medium, transverse to the axes of fibers (assumed parallel cylinders) and the shear straining along the fibers. As shown by Hashin [HAh, Chapter 5.5.1], the appropriate effective parameters coincide, due to the same governing equations for these two phenomena.

Much more nontrivial cross-properties relations are however those where there is no direct mathematical analogy, and the relations result from the same underlying internal structure of the medium. Here we shall present only the first and maybe the most famous relation of this kind—the so-called *Levin formula* which ties the effective thermal expansion coefficient with the bulk modulus of a two-phase solid [LEa].

Following Levin himself [LEa], consider two types of straining of a thermoelastic solid: the first, due to given surface traction at fixed temperature, the other—due to temperature change with no such tractions.

More specifically, let $\boldsymbol{\varepsilon}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ be the strain and stress fields that appear in the volume \mathcal{V} at fixed temperature $T = 0$ and under the homogeneous boundary conditions (2.58). These conditions imply

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^0, \quad \bar{\boldsymbol{\varepsilon}} = \mathbb{M}^* : \boldsymbol{\sigma}^0, \quad (3.69)$$

cf. Lemma 2.7, where \mathbb{M}^* is the effective compliance tensor of the medium.

Consider a second pair of strain and stress fields in the medium, $\boldsymbol{\varepsilon}^{(t)}(\boldsymbol{x})$ and $\boldsymbol{\sigma}^{(t)}(\boldsymbol{x})$, due solely to the change T of the temperature, with no boundary tractions; let $\boldsymbol{u}^{(t)}(\boldsymbol{x})$ be the appropriate displacement field. These fields appear as a consequence of the inhomogeneity of the thermal expansion coefficient $\alpha(\boldsymbol{x})$ which takes the different values, α_1 and α_2 , in the phases ‘1’ and ‘2’ respectively. According

to the basic thermoelastic law, we have

$$\boldsymbol{\varepsilon}^{(t)}(\mathbf{x}) = \mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}^{(t)}(\mathbf{x}) + \alpha(\mathbf{x})T\mathbf{I}. \quad (3.70)$$

Moreover,

$$\overline{\boldsymbol{\varepsilon}^{(t)}} = \frac{1}{V} \int_{\mathcal{V}} \boldsymbol{\varepsilon}^{(t)}(\mathbf{x}) \, d\mathbf{x} = \alpha^*T\mathbf{I}, \quad (3.71)$$

which is just the definition of the *effective thermal expansion coefficient* α^* of the medium (having assumed, for simplicity's sake, isotropy of thermal expansion effects as well).

Note first the identity

$$\begin{aligned} \frac{1}{V} \int_{\mathcal{V}} \boldsymbol{\sigma}(\mathbf{x}) : \boldsymbol{\varepsilon}^{(t)}(\mathbf{x}) \, d\mathbf{x} &= \frac{1}{V} \int_{\mathcal{V}} \nabla \cdot (\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{u}^{(t)}(\mathbf{x})) \, d\mathbf{x} \\ &= \frac{1}{V} \int_{\mathcal{S}} \mathbf{n} \cdot \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{u}^{(t)}(\mathbf{x}) \, dS = \boldsymbol{\sigma}^0 : \overline{\boldsymbol{\varepsilon}^{(t)}} = \alpha^*T \operatorname{Tr} \boldsymbol{\sigma}^0, \end{aligned} \quad (3.72)$$

which easily follows from Gauss' theorem, the boundary conditions (2.55), the self-equilibrium of the field $\boldsymbol{\sigma}(\mathbf{x})$ and the definition (3.71) of the effective thermal expansion constant.

The second identity that we shall need reads

$$\int_{\mathcal{V}} \boldsymbol{\sigma}^{(t)}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \, d\mathbf{x} = \int_{\mathcal{V}} \boldsymbol{\sigma}^{(t)}(\mathbf{x}) : \mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) \, d\mathbf{x} = 0, \quad (3.73)$$

since the field $\boldsymbol{\sigma}^{(t)}(\mathbf{x})$ is “temperature-induced,” with no surface tractions involved, cf. the derivation of (3.72).

Introduce now the Hooke law (3.70) into the first integral of (3.72)

$$\begin{aligned} \frac{1}{V} \int_{\mathcal{V}} \boldsymbol{\sigma}(\mathbf{x}) : [\mathbb{M}(\mathbf{x}) : \boldsymbol{\sigma}^{(t)}(\mathbf{x}) + \alpha(\mathbf{x})T\mathbf{I}] \, d\mathbf{x} \\ = \frac{1}{V} T \int_{\mathcal{V}} \alpha(\mathbf{x}) \operatorname{Tr} \boldsymbol{\sigma}(\mathbf{x}) \, d\mathbf{x} = \alpha^*T \operatorname{Tr} \boldsymbol{\sigma}^0, \end{aligned} \quad (3.74)$$

having used (3.73). Since $\alpha(\mathbf{x})$ is step-constant, Eq. (3.74) gives

$$\alpha_1 \phi_1 \langle \operatorname{Tr} \boldsymbol{\sigma} \rangle_1 + \alpha_2 \phi_2 \langle \operatorname{Tr} \boldsymbol{\sigma} \rangle_2 = \alpha^* \operatorname{Tr} \boldsymbol{\sigma}^0. \quad (3.75)$$

It remains to combine now (3.75) with the obvious formulae

$$\operatorname{Tr} \boldsymbol{\sigma}^0 = \phi_1 \langle \operatorname{Tr} \boldsymbol{\sigma} \rangle_1 + \phi_2 \langle \operatorname{Tr} \boldsymbol{\sigma} \rangle_2,$$

$$\operatorname{Tr} \boldsymbol{\varepsilon}^0 = \phi_1 \langle \operatorname{Tr} \boldsymbol{\varepsilon} \rangle_1 + \phi_2 \langle \operatorname{Tr} \boldsymbol{\varepsilon} \rangle_2,$$

$$\operatorname{Tr} \boldsymbol{\sigma}^0 = 3k^* \operatorname{Tr} \boldsymbol{\varepsilon}^0, \quad \langle \operatorname{Tr} \boldsymbol{\sigma} \rangle_i = 3k_i \langle \operatorname{Tr} \boldsymbol{\varepsilon} \rangle_i, \quad i = 1, 2,$$

cf. Eq. (2.35), which allow to exclude all the traces of the stress and strain tensors. The final result reads

$$\alpha^* = \frac{\alpha_2(1/k^* - 1/k_1) - \alpha_1(1/k^* - 1/k_2)}{1/k_2 - 1/k_1} \quad (3.76)$$

and this is just the Levin formula.

Remark 3.9 *Almost at the same time Levin's formula was rediscovered and generalized by Rosen [ROb], Shapery [SHa] et al., see also [ROc], [KRb] and the book [CHd, Chapters 9.3 and 9.4]. The general "philosophy" of deriving various cross-properties relations was recently developed and implemented by Grabovsky and Milton [GRa], [MIf]. Torquato and co-authors have discovered another class of very interesting and unexpected such relations, involving, e.g. fluid permittivity of a medium; details and references can be found again in Torquato's survey in the present volume (Chapter 2).*

1.3.7 The Elementary Bounds on the Effective Absorption Coefficient

The variational principles of classical type for the absorption problem (2.66) can be easily formulated, together with their modification [TA b]. Other more refined variational procedures in the hard limit (2.69), that corresponds to the Smoluchowski problem, are presented in Torquato's survey in this volume. Here we shall only derive the elementary estimates of Wiener's type on the effective rate constant k^{*2} without engaging directly variational arguments. The reasoning that follows is a reminiscent of a Beran's one for the conductivity case [BEh].

Let us multiply both sides of Eq. (2.66) by $c(\mathbf{x})$ and average the result over the volume \mathcal{V} :

$$K\bar{c} = \frac{1}{V} \int_{\mathcal{V}} [|\nabla c(\mathbf{x})|^2 + k^2(\mathbf{x})c^2(\mathbf{x})] d\mathbf{x}, \quad (3.77)$$

having used that

$$\int_{\mathcal{V}} c \Delta c d\mathbf{x} = - \int_{\mathcal{V}} |\nabla c|^2 d\mathbf{x},$$

in virtue of the boundary condition (2.67). Let $c(\mathbf{x}) = \bar{c} + c'(\mathbf{x})$, so that $c'(\mathbf{x})$ is the fluctuating part of $c(\mathbf{x})$, $\overline{c'} = 0$. Then

$$\begin{aligned} K\bar{c} &= \frac{1}{V} \int_{\mathcal{V}} \left\{ |\nabla c'(\mathbf{x})|^2 + k^2(\mathbf{x}) \left[\bar{c}^2 + 2\bar{c}c'(\mathbf{x}) + |c'(\mathbf{x})|^2 \right] \right\} d\mathbf{x} \\ &\geq \bar{k}^2 \bar{c}^2 + \frac{2\bar{c}}{V} \int_{\mathcal{V}} k^2(\mathbf{x}) [c(\mathbf{x}) - \bar{c}] d\mathbf{x} = -\bar{k}^2 \bar{c}^2 + 2\bar{c} \overline{k^2(\mathbf{x})c(\mathbf{x})} \end{aligned}$$

i.e. $\bar{k}^2 \bar{c} \geq K = k^{*2} \bar{c}$. In virtue of Eq. (2.70), we thus have

$$\begin{aligned} \bar{k}^2 \bar{c} \geq K = k^{*2} \bar{c}, \quad \text{i.e.} \quad k^{*2} \leq k_v^2, \\ k_v^2 = \bar{k}^2 = \phi_1 k_1^2 + \phi_2 k_2^2. \end{aligned} \tag{3.78}$$

Fully similar manipulations, omitted here, lead to the conclusion that the Reuss type approximation k_r^2 , defined as

$$\frac{1}{k_r^2} = \frac{\phi_1}{k_1^2} + \frac{\phi_2}{k_2^2}, \tag{3.79}$$

provides a lower bound on the effective absorption coefficient. Together with Eq. (3.77), this means that

$$k_r^2 \leq k^{*2} \leq k_v^2, \tag{3.80}$$

whatever the (macroscopically isotropic) internal constitution of the medium. This conclusion is obviously the exact absorption counterpart of the Wiener (3.29) or Hill's (3.64) bounds in the scalar and elastic contexts, respectively.

Similarly to these bounds, the estimates (3.80) are also sharp, in the sense that they *cannot* be improved (see Section 1.5.7). However, the particular constitution which realize the bounds (more precisely, approximate them as closely as we wish), are here isotropic. Therefore, the fact that a binary mixture is macro-isotropic, does not allow us to narrow (3.80) for given volume fractions, unlike the scalar conductivity case treated in Section 1.3.4. Bounds of Hashin-Shtrikman's type here also exists but the full two-point correlation function enters them through a certain integral parameter, see [TA] and also the recent author's paper [MA] for details.

1.4 The Single Inclusion Problem

In this Section the so-called *single inclusion problem* is treated. It concerns determination of temperature and/or displacement fields in a solid, containing an inhomogeneity whose thermal and/or elastic properties differ from those of the surrounding medium. Having in mind the application to heterogeneous solids, the main interest for us is the temperature and/or displacement gradient *within* the inhomogeneity. This gradient turns out to be constant for ellipsoidal shape. The most important particular cases—sphere, fiber, layer or disk—are elaborated as examples and explicit results are listed first in conductivity and then in elastic contexts.

The application of the obtained results will be postponed until Section 1.5. There they will serve as a basic building block when deriving approximate formulae for the effective properties of heterogeneous media.

1.4.1 Scalar Conductivity—Integral Equation

Consider an infinite body (matrix), with the conductivity tensor \mathbf{K}_1 , containing an inhomogeneity \mathcal{W} (a filler particle), with a different conductivity tensor \mathbf{K}_2 . For the moment both tensors \mathbf{K}_1 and \mathbf{K}_2 are symmetric second-rank tensors, though the main attention in what follows will be concentrated on the isotropic case when $\mathbf{K}_i = \kappa_i \mathbf{I}$, $i = 1, 2$. The conductivity field of the inhomogeneous solid under study is

$$\mathbf{K}(\mathbf{x}) = \mathbf{K}_1 + [\mathbf{K}]h_w(\mathbf{x}), \quad [\mathbf{K}] = \mathbf{K}_2 - \mathbf{K}_1, \quad (4.1)$$

where $h_w(\mathbf{x})$ is the characteristic function of the inhomogeneity \mathcal{W} . At the absence of body sources, the temperature field $\theta(\mathbf{x})$ in the solid obeys the equation

$$\nabla \cdot \{\mathbf{K}_1 \cdot \nabla \theta(\mathbf{x})\} + \nabla \cdot \{h_w(\mathbf{x})[\mathbf{K}] \cdot \nabla \theta(\mathbf{x})\} = 0, \quad (4.2)$$

as it follows from Eqs. (1.5) and (4.1).

Let $G(\mathbf{x})$ be the Green function for the matrix, i.e.

$$\nabla \cdot \{\mathbf{K}_1 \cdot \nabla G(\mathbf{x})\} + \delta(\mathbf{x}) = 0,$$

which represents the temperature field, generated by a (unit) point source, located at the origin $\mathbf{x} = 0$. The Green function allows us to recast Eq. (4.2) as

$$\theta(\mathbf{x}) = \theta^\infty(\mathbf{x}) + \int G(\mathbf{x} - \mathbf{x}') \nabla \cdot \{h_w(\mathbf{x}')[\mathbf{K}] \cdot \nabla \theta(\mathbf{x}')\} d\mathbf{x}' \quad (4.3)$$

(the integral is over the whole \mathcal{R}^3), or

$$\nabla \theta(\mathbf{x}) = \nabla \theta^\infty(\mathbf{x}) + \int_{\mathcal{W}} \mathbf{\Gamma}(\mathbf{x} - \mathbf{x}') \cdot [\mathbf{K}] \cdot \nabla \theta(\mathbf{x}') d\mathbf{x}', \quad (4.4)$$

where

$$\mathbf{\Gamma}(\mathbf{x}) = \nabla \nabla G(\mathbf{x}). \quad (4.5)$$

Eq. (4.4) is the basic integral equation which governs the temperature gradient in the solid with a single inhomogeneity, provided the temperature gradient at infinity is prescribed. In the elasticity context it has been derived by a number of authors, see, e.g. [KUb]. Note, however, that the kernel $\mathbf{\Gamma}(\mathbf{x})$ has the singularity $|\mathbf{x}|^{-3}$ at $|\mathbf{x}| \rightarrow 0$, so that the integration in Eq. (4.4) should be understood in the sense of generalized functions, see [KUa].

1.4.2 Scalar Conductivity—Ellipsoidal Inhomogeneity

As seen from the analysis of Section 1.2.6 and the definition of the concentration factors, the main interest when modelling effective conductivity of heterogeneous media, is the temperature gradient within the inhomogeneity \mathcal{W} . The latter can be easily found from the integral equation (4.4) for ellipsoidal inhomogeneities directly, without using the elegant but longer considerations of Eshelby [ESa], concerned with the eigenstrains and eigenstresses in an inclusion. The reasoning to be used follows the basic idea, sketched very concisely by Wu [WUa]. (More details and many particular cases have been explicitly treated by the author later on [MAd].)

Let $\mathbf{G}^\infty = \nabla \theta^\infty(\mathbf{x})$ be a constant vector; it is easily seen that a simple solution of Eq. (4.4) within \mathcal{W} can be found, if the temperature gradient $\nabla \theta(\mathbf{x})$ is also constant in \mathcal{W} . To simplify the technical details, assume that the matrix is isotropic. Then

$$G(\mathbf{x}) = \frac{1}{4\pi\kappa_1|\mathbf{x}|}. \quad (4.6)$$

The field $\nabla\theta(\mathbf{x})$ will be constant in \mathcal{W} if and only if

$$\mathbf{P}(\mathbf{x}) = - \int_{\mathcal{W}} \boldsymbol{\Gamma}(\mathbf{x} - \mathbf{x}') d\mathbf{x}' = - \frac{1}{\kappa_1} \nabla \nabla \varphi_w(\mathbf{x}) \quad (4.7)$$

is constant within the inhomogeneity \mathcal{W} . Here

$$\varphi_w(\mathbf{x}) = \int_{\mathcal{W}} \frac{d\mathbf{x}'}{4\pi|\mathbf{x} - \mathbf{x}'|} \quad (4.8)$$

denotes the Newtonian potential for the region \mathcal{W} . Recall that the latter solves the equation

$$\Delta\varphi_w(\mathbf{x}) + h_w(\mathbf{x}) = 0, \quad (4.9)$$

which will be used repeatedly in what follows.

Thus, to have a simple solution of Eq. (4.4), the potential $\varphi_w(\mathbf{x})$ should be a quadratic function within \mathcal{W} , which is true if \mathcal{W} is ellipsoidal [ESa], [MUa]. Therefore, if the temperature gradient is constant at infinity and the matrix is isotropic, this gradient is also constant within *any* ellipsoidal inhomogeneity, whatever the anisotropy (i.e. the tensor \mathbf{K}_2) of the latter.¹¹ That is why, Eq. (4.4) implies

$$\begin{aligned} \nabla\theta(\mathbf{x}) &= \langle \nabla\theta(\mathbf{x}) \rangle_w = \frac{1}{W} \int_{\mathcal{W}} \nabla\theta(\mathbf{x}') d\mathbf{x}' = \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot \mathbf{G} \\ \mathbf{A}_w(\kappa_1, \mathbf{K}_2) &= \left(\mathbf{I} + \mathbf{P} \cdot [\mathbf{K}] \right)^{-1}, \end{aligned} \quad (4.10)$$

$$[\mathbf{K}] = \mathbf{K}_2 - \kappa_1 \mathbf{I}, \quad \mathbf{x} \in \mathcal{W}.$$

The tensor \mathbf{A}_w , that appeared in Eq. (4.10), plays a central role in the elementary models of composite media, as it will be seen below. That is why we shall specify it now for the ellipsoidal shape of \mathcal{W} and its particular cases—sphere, fiber, layer or disk.

¹¹This fact holds true for an anisotropic matrix as well. We shall not consider however such a matrix, since the technical details are cumbersome, even in the scalar context. Moreover, both in scalar conductivity and elasticity contexts, the “polynomial conservation” property holds. This means that if the applied temperature gradient or strain field at infinity is a polynomial of a degree n , these fields are *also* polynomials, of the *same* degree n , within the ellipsoidal inhomogeneity; see [KUb] or [KUa, Section 4.9].

- Let \mathcal{W} be a *sphere*. The potential $\varphi_w(\mathbf{x})$ is spherically symmetric then, so that $\nabla\nabla\varphi_w(\mathbf{x}) = \alpha\mathbf{I}$ is an isotropic tensor, $\forall\mathbf{x} \in \mathcal{W}$. Making a contraction and invoking Eq. (4.9), one finds $\alpha = 1/3$, i.e.

$$\nabla\nabla\varphi_w(\mathbf{x}) = -\frac{1}{3}\mathbf{I}, \quad \mathbf{P} = \frac{1}{3\kappa_1}\mathbf{I}, \quad \mathbf{x} \in \mathcal{W}, \quad (4.11)$$

and thus

$$\mathbf{A}_w(\kappa_1, \mathbf{K}_2) = \left(\mathbf{I} + \frac{1}{3\kappa_1}[\mathbf{K}] \right)^{-1}. \quad (4.12)$$

If the inhomogeneity is also isotropic, then $\mathbf{K}_2 = \kappa_2\mathbf{I}$ and Eq. (4.12) yields the already known result (1.14), (1.15),

$$\mathbf{A}_w(\kappa_1, \kappa_2) = \gamma\mathbf{I}, \quad \gamma = \frac{3\kappa_1}{\kappa_2 + 2\kappa_1} \quad (\text{sphere}), \quad (4.13)$$

found directly in Section 1.1.4.

- Let the inhomogeneity be a *circular fiber* along the axis x_3 . The potential $\varphi_w(\mathbf{x})$ then depends on the x_1, x_2 coordinates only and the same symmetry arguments, as those utilized above for the sphere, give

$$\nabla\nabla\phi_w(\mathbf{x}) = -\frac{1}{2}(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2), \quad \mathbf{P} = \frac{1}{2}\kappa_1(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2), \quad (4.14)$$

$\mathbf{x} \in \mathcal{W}$. Hence, for an isotropic fiber,

$$\mathbf{A}_w = \frac{2\kappa_1}{\kappa_1 + \kappa_2}(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2) + \mathbf{e}_3\mathbf{e}_3 \quad (\text{fiber}). \quad (4.15)$$

- Let the inhomogeneity be a *layer* $-h \leq x_3 \leq h$, perpendicular to the x_3 -axis. The potential $\varphi_w(\mathbf{x})$ then depends on x_3 solely, so that $\varphi_{,ij} = -\delta_{3i}\delta_{3j}$, i.e.

$$\nabla\nabla\varphi_w(\mathbf{x}) = -\mathbf{e}_3\mathbf{e}_3, \quad \mathbf{P} = \frac{1}{\kappa_1}\mathbf{e}_3\mathbf{e}_3, \quad \mathbf{x} \in \mathcal{W}, \quad (4.16)$$

and hence, for an isotropic layer,

$$\mathbf{A}_w = \mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2 + \frac{\kappa_1}{\kappa_2}\mathbf{e}_3\mathbf{e}_3 \quad (\text{layer}). \quad (4.17)$$

Remark 4.1 The tensors \mathbf{A}_w for the simplest shapes, treated until now (sphere, fiber and layer), can be extracted as particular cases of the more general result below, valid for an arbitrary spheroid \mathcal{W} . However, the evaluation of \mathbf{A}_w in these cases is extremely simple, utilizing obvious symmetry arguments for the potentials' gradients in the appropriate regions; the use of the classical, but not that elementary formula (4.20) below, is totally avoided in this way. The same remark holds true for the elastic case, as we shall see in the next subsection.

- Let the inhomogeneity \mathcal{W} be an ellipsoid with the semiaxes a , b and c along the Cartesian axes x_1 , x_2 and x_3 , respectively. Then

$$\nabla\nabla\varphi_w(\mathbf{x}) = -(M_1\mathbf{e}_1\mathbf{e}_1 + M_2\mathbf{e}_2\mathbf{e}_2 + M_3\mathbf{e}_3\mathbf{e}_3), \quad \mathbf{x} \in \mathcal{W}, \quad (4.18)$$

where \mathbf{e}_i are the unit vectors along the axes x_i , $i = 1, 2, 3$.

The coefficients M_i in the latter formula are often called in the physical literature *depolarizations* (the quantities $4\pi M_i$ in magnetic theory are referred to as *demagnetizing factors*). They have been extensively tabulated, see, e.g. [BRe, p. 28]. Obviously

$$M_1 + M_2 + M_3 = 1,$$

as it follows from Eq. (4.9). The factors M_i are expressed as the classical elliptical integrals, cited here for the sake of completeness:

$$M_1 = \frac{1}{2}abc \int_0^\infty \frac{du}{(a^2 + u)\sqrt{(a^2 + u)(b^2 + u)(c^2 + u)}}, \quad (4.19)$$

and similarly for M_2 and M_3 with a cyclic change $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$. A clear and concise derivation of (4.19), using the appropriate ellipsoidal coordinate system, can be found in the opening pages of Landau and Lifshitz's book [LAa], see also the book of Stratton [STa, pp. 207–215, 257–258].

- For our purposes it suffices however to consider only *spheroids*, i.e. *rotational ellipsoids* with the semiaxes $a = b \neq c$. Then

$$M_\perp = M_1 = M_2 = \frac{1}{2}a^2c \int_0^\infty \frac{du}{(a^2 + u)^2\sqrt{c^2 + u}},$$

$$M = M_3 = \frac{1}{2}a^2c \int_0^\infty \frac{du}{(a^2 + u)(c^2 + u)^{3/2}}.$$

Both integrals can be elementary evaluated:

$$M = \begin{cases} \frac{1}{e^2} \left(1 - \frac{\sqrt{1-e^2}}{e} \arcsin e \right), & \text{if } c < a \quad (\text{oblate}), \\ \frac{1-e^2}{2e^3} \left(\ln \frac{1+e}{1-e} - 2e \right), & \text{if } c > a \quad (\text{prolate}), \end{cases} \quad (4.20)$$

$$M_{\perp} = \frac{1}{2}(1-M), \quad \xi = \begin{cases} c/a, & \text{if } c < a \quad (\text{oblate}), \\ a/c, & \text{if } c > a \quad (\text{prolate}), \end{cases}$$

$e = \sqrt{1-\xi^2}$ is the eccentricity of the ellipsoid, see again the book [LAa]. The type of the spheroid is indicated as well in Eq. (4.20).

If both *matrix and inhomogeneity are isotropic*, Eqs. (4.10) and (4.20) yield

$$\begin{aligned} \mathbf{A}_w(\kappa_1, \kappa_2) &= \left(\mathbf{I} + \mathbf{P} \cdot [\mathbf{K}] \right)^{-1} = \left(\mathbf{I} - \frac{[\kappa]}{\kappa_1} \nabla \nabla \phi_w \right)^{-1} \\ &= \left[\mathbf{I} + \frac{[\kappa]}{\kappa_1} \left(M_{\perp} (\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) + M \mathbf{e}_3 \mathbf{e}_3 \right) \right]^{-1} \\ &= \left[\left(1 + \frac{[\kappa]}{\kappa_1} M_{\perp} \right) (\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) + \left(1 + \frac{[\kappa]}{\kappa_1} M \right) \mathbf{e}_3 \mathbf{e}_3 \right]^{-1}, \end{aligned}$$

since $\mathbf{I} = \mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2 + \mathbf{e}_3 \mathbf{e}_3$. Thus

$$\begin{aligned} \mathbf{A}_w(\kappa_1, \kappa_2) &= \frac{\kappa_1}{\kappa_1 + [\kappa] M_{\perp}} (\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) \\ &\quad + \frac{\kappa_1}{\kappa_1 + [\kappa] M} \mathbf{e}_3 \mathbf{e}_3 \quad (\text{spheroid}). \end{aligned} \quad (4.21)$$

Remark 4.2 *The above considered, in an elementary way, cases of a sphere, fiber and layer, can be easily extracted from the general formula (4.21). Indeed, in these cases $\xi = c/a = 1$, $\xi \rightarrow \infty$ and $\xi \rightarrow 0$, respectively, i.e. the spheroid is a sphere or degenerates into a fiber or a flat disk (layer). The depolarization factors M_{\perp} and M , defined in Eq. (4.20), then become*

$$\begin{aligned} M_{\perp} &= M = \frac{1}{3} && (\text{sphere}), \\ M_{\perp} &= \frac{1}{2}, \quad M = 0 && (\text{fiber}), \\ M_{\perp} &= 0, \quad M = 1 && (\text{disk}). \end{aligned} \quad (4.22)$$

When inserting these values in (4.21), the particular cases (4.13), (4.17), (4.15) will immediately appear one after another.

- Let the spheroid be randomly (and uniformly) oriented, then

$$\begin{aligned} \langle \mathbf{A}_w \rangle_\Omega &= \gamma_\Omega \mathbf{I}, \\ \gamma_\Omega &= \frac{1}{3} \left(\frac{2\kappa_1}{\kappa_1 + [\kappa]M_\perp} + \frac{\kappa_1}{\kappa_1 + [\kappa]M} \right), \end{aligned} \quad (4.23)$$

where $\langle \mathbf{A}_w \rangle_\Omega$ denotes the value of the tensor \mathbf{A}_w averaged with respect to all possible orientations of the axes x_i ; in deriving Eq. (4.23) we have used that the tensor $\langle \mathbf{A}_w \rangle_\Omega$ should obviously be isotropic.

Note that the above mentioned limiting cases $\xi = c/a \rightarrow \infty$ and $\xi \rightarrow 0$, when combined with the previous formula (4.23), can be interpreted as the situations, in which the inclusion is either a *randomly oriented needle* or a *randomly oriented disk*, respectively. Using Eq. (4.22) in (4.23) yields the simple formulae in these two cases

$$\begin{aligned} \langle \mathbf{A}_w \rangle_\Omega &= \frac{5\kappa_1 + \kappa_2}{3(\kappa_1 + \kappa_2)} \mathbf{I} \quad (\text{needle}), \\ \langle \mathbf{A}_w \rangle_\Omega &= \frac{\kappa_1 + 2\kappa_2}{\kappa_2} \mathbf{I} \quad (\text{disk}). \end{aligned} \quad (4.24)$$

Remark 4.3 *The foregoing analysis concentrated on the temperature gradient within the ellipsoidal inclusion, i.e. on the tensor \mathbf{A}_w , defined in Eq. (4.10). However, once the tensor \mathbf{A}_w is known the temperature field outside the inclusion can be immediately found, using the integral equation (4.3). Indeed, for an isotropic matrix, with the Green function given in (4.6), this equation yields*

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} + \frac{1}{\kappa_1} \nabla \varphi_w(x) \cdot [\mathbf{K}] \cdot \mathbf{A}_w \cdot \mathbf{G} \quad (4.25)$$

after an obvious integration by parts. If the gradients of both sides of (4.25) are taken, the result will reproduce the formula (4.10) for the tensor \mathbf{A}_w , provided $\mathbf{x} \in \mathcal{W}$.

1.4.3 Singular Inclusions and Nonideal Contacts

The assumption of ideal contact between the phases, adopted until now, is a starting point in the great majority of works on heterogeneous media. Under this idealization, the temperature field and the normal component of the heat flux are to be continuous at phase interfaces. Imperfect interfaces are however a fact in many circumstances and reflect themselves either in a discontinuity of the temperature field or of the normal component of the heat flux. More details can be found in the papers, cited below and in the references they contain.

1.4.3.1 Singular Inclusions

A convenient way to treat nonideal contacts is based on the notion of *singular inclusions*, as introduced by Kanaun [KAc], see also the earlier paper [SOa]. Though in [KAc] the elasticity context was used, the underlying idea is simple, appealing and general.¹²

Let one of the inclusion's dimensions be of the order δ , small as compared to the other two. Let, at the same time, its material property like conductivity κ_s or resistivity $k_s = 1/\kappa_s$ be of the order $1/\delta$. Then the limit $\delta \rightarrow 0$ produces the two models of a singular inclusion.

In the first model $\kappa_s \rightarrow \infty$, being of the order $1/\delta$, as $\delta \rightarrow 0$. Then the limit

$$C^I = \frac{1}{a\kappa_1} \lim_{\substack{\delta \rightarrow 0 \\ \kappa_s \rightarrow \infty}} \delta \kappa_s \quad (4.26)$$

remains *finite*. Here, to make C^I dimensionless, the conductivity κ_1 of the matrix is employed, together with a certain characteristic size, a , of the inclusion under study. For simplicity sake, we assume that $C^I = \text{const}$, though in general C^I can be an arbitrary function, defined on the surface of the inclusion Σ . (To this end it suffices to take the inclusion inhomogeneous, with conductivity $\kappa_s = K(\boldsymbol{x})/\delta + \mathcal{O}(1)$ as $\delta \rightarrow 0$, where $K(\boldsymbol{x})$ is a prescribed function on this surface.)

¹²In a particular case, the same idea was formulated clearly by Pham Huy and Sanchez-Palencia [PHa]. The authors treated conductivity problems in the presence of a superconducting singular inclusion (in the terminology introduced below, see (4.26)) and proved the appropriate existence theorems using functional analysis arguments. Note that one of the motivation of [PHa] came, in particular, from a diffraction problem, where the electromagnetic wave field is disturbed by the presence of a very thin screen, possessing very high electric conductivity.

The so-obtained singular inclusion can be called “superconducting.” The temperature remains continuous everywhere, but the heat flux suffers a jump when crossing its surface Σ . We shall illustrate these facts below, when treating nonideal contact of a spherical inhomogeneity in a matrix.

In the elastic context the superconducting inclusion is somewhat similar to a rigid “flake” (membrane) in the medium. The displacement is continuous, but the normal stress component has a jump on the flake. An integral equation on the surface Σ , which specifies the stress field in an unbounded elastic medium with such an inclusion, has been derived by Kanaun [KA_c].

In the second model the resistivity $k_s = 1/\kappa_s \rightarrow \infty$, being of the order $1/\delta$, as $\delta \rightarrow 0$. Then the limit

$$C^{\text{II}} = \frac{1}{ak_1} \lim_{\substack{\delta \rightarrow 0 \\ k_s \rightarrow \infty}} \delta k_s \quad (4.27)$$

remains *finite*. Here, to make C^{II} dimensionless, the compliance k_1 of the matrix is employed; again a is a certain characteristic size of the inclusion. Once more we have assumed, for simplicity, that $C^{\text{II}} = \text{const}$, though in general it can be an arbitrary function, defined on the surface of the inclusion Σ . (See the comment after Eq. (4.26).)

The so-obtained singular inclusion can be called “resisting.” Here the heat flux remains continuous, but the temperature suffers a jump when crossing the surface Σ . Again, we shall illustrate these facts below, when treating the appropriate nonideal contact of a spherical inhomogeneity in a matrix.

In the elastic context the resisting inclusion is somewhat similar to a crack. (The reader should be warned that the crack itself, as treated in solid mechanics, is only a special particular case of the inclusion under study, see [KA_c].) The displacement has a jump, but the normal stress component is continuous on Σ . An integral equation on the surface Σ , which specifies the strain field in an unbounded elastic medium with such an inclusion, has been also derived by Kanaun [KA_c].

1.4.3.2 Nonideal Contacts

After Kanaun *et al.* [KA_d], [KA_e], we shall treat nonideal contacts as singular inclusions, spread over the surface of a bulk inhomogeneity.

For an illustration consider, following Torquato and Rintoul [TOd], the simplest case of a spherical inhomogeneity of radius a and conductivity κ_2 . It is coated with a thin concentric layer with thickness δ and conductivity κ_s , such that $\delta \ll a$, $\kappa_s \gg \kappa_1$. The so-obtained “composite” sphere is then immersed into a homogeneous matrix of conductivity κ_1 . The distinguished limit is just (4.26), with a *finite* $C = C^I$. This is the definition of the “superconducting” interphase, as adopted in [TOd]. Obviously, such an interphase is nothing but a superconducting singular inclusion, spread over the surface $r = a$ of the spherical inhomogeneity.

In the second case let the conductivity of the thin layer κ_s be vanishingly small. The distinguished limit is now (4.27), which we shall write, after Torquato and Rintoul [TOd], in the equivalent form

$$R = \frac{\kappa_2}{a} \lim_{\substack{\delta \rightarrow 0 \\ \kappa_s \rightarrow 0}} \frac{\delta}{\kappa_s}, \quad (4.28)$$

with a *finite* R . This is the definition of the “resistive” interphase [TOd]. Again it is clear that such an interphase is nothing but a resisting singular inclusion, spread over the surface $r = a$ of the spherical inhomogeneity.

1.4.3.3 The “Superconducting” Spherical Inhomogeneity

Consider a spherical inhomogeneity with a “superconducting” interphase. At infinity, the same condition as in Eq. (1.7) applies, i.e. $\theta(\mathbf{x}) \rightarrow \mathbf{G} \cdot \mathbf{x}$ as $|\mathbf{x}| \rightarrow \infty$.

The solution of such a single inclusion problem is very simple due to the assumed spherical shape. (For the ellipsoidal shape the problem is much more complicated and the full analytical solution has been only recently given by Miloh and Benveniste [MIa].) Indeed, consider, before passing to the limit (4.26), the above composite sphere. The temperature field has the form (1.9), with

$$\varphi(r) = \begin{cases} \frac{1}{2}C_1 r^2, & \text{if } r < a, \\ \frac{1}{2}C_2 r^2 - C_3 \frac{a^3}{r}, & \text{if } a < r < b, \\ \frac{1}{2}r^2 - C_4 \frac{a^3}{r}, & \text{if } b < r < \infty, \end{cases} \quad (4.29)$$

where $b = a + \delta$. The continuity of $\theta(\mathbf{x})$ and $d\theta/dr$ at $r = a$ and $r = b$ implies the following system for the unknowns C_1 to C_4 :

$$\begin{aligned} C_1 &= C_2 + C_3, \\ C_2 + \left(\frac{a}{b}\right)^3 C_3 &= 1 + \left(\frac{a}{b}\right)^3 C_4, \\ \kappa_2 C_1 &= \kappa_s(C_2 - 2C_3), \\ \kappa_s \left(C_2 - 2 \left(\frac{a}{b}\right)^3 C_3 \right) &= \kappa_1 \left(1 - 2 \left(\frac{a}{b}\right)^3 C_4 \right), \end{aligned} \tag{4.30}$$

cf. Eqs. (1.12) and (1.13).

In the superconducting case under discussion, the solution of (4.28) has the form

$$C_k = C_k^0 + \mathcal{O}\left(\frac{\delta}{a}\right), \quad k = 1, \dots, 4.$$

In the limit $\kappa_s \rightarrow \infty$, the first three of the equations (4.30) give

$$C_2^0 + C_3^0 = 1 + C_4^0, \quad C_2^0 = 2C_3^0, \quad C_1^0 = 3C_3^0. \tag{4.31}$$

Note next that

$$\left(\frac{a}{b}\right)^3 = 1 - 3\frac{\delta}{a} + \mathcal{O}\left(\frac{\delta}{a}\right), \tag{4.32}$$

(since $\delta = b - a$) which, when employed in the last of the equations (4.30), yields

$$\kappa_2 C_1^0 + 6\kappa_1 C C_3^0 = \kappa_1(1 - 2C_4^0), \tag{4.33}$$

having taken the limit (4.26), with (4.31) taken into account, and recalling that $C = C^I$.

The relations (4.31) and (4.33) specify the needed constants C_1^0 to C_4^0 in the superconducting limit:

$$\begin{aligned} C_1^0 &= \frac{3\kappa_1}{\kappa_2 + 2(1+C)\kappa_1}, \quad C_2^0 = 2C_1/3, \\ C_3^0 = C_1/3, \quad C_4^0 = C_1^0 - 1 &= \frac{\kappa_1(1-2C) - \kappa_2}{\kappa_2 + 2(1+C)\kappa_1}. \end{aligned} \tag{4.34}$$

Hence, in the conductance case under study, the solution of the spherical inclusion problem has the same form (1.14) as that for the ideal contact, cf. Eq. (1.14), namely,

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} \begin{cases} \gamma^s, & \text{if } |\mathbf{x}| < a, \\ 1 - \beta^s (a/r)^3, & \text{if } |\mathbf{x}| > a, \end{cases} \quad (4.35)$$

with the constants

$$\gamma^s = C_1^0 = 1 - \beta^s = \frac{3\kappa_1}{\kappa_2 + 2(1+C)\kappa_1}, \quad \beta^s = -C_4^0. \quad (4.36)$$

The temperature field (4.35) is obviously continuous at the inclusion surface $r = a$, but the heat flux suffers a jump in this case

$$[q_n] \Big|_{r=a} \neq 0, \quad [q_n] \Big|_{r=a} = \kappa_1 \frac{\partial \theta}{\partial r} \Big|_{r=a+0} - \kappa_2 \frac{\partial \theta}{\partial r} \Big|_{r=a-0}.$$

Its value can be easily found, using Eqs. (4.35) and (4.36):

$$\begin{aligned} [q_n] \Big|_{r=a} &= \left(\kappa_1(1 + 2\beta^s) - \kappa_2\gamma^s \right) \mathbf{G} \cdot \mathbf{e}_r \\ &= \frac{6\kappa_1^2 C}{\kappa_2 + 2(1+C)\kappa_1} \mathbf{G} \cdot \mathbf{e}_r. \end{aligned} \quad (4.37)$$

The surface concentration factor $\mathbf{A}_s^{(12)}$, for a single sphere (we underline this adding the subscript ‘s’), can be now easily evaluated:

$$\begin{aligned} \mathbf{q}^{(12)} &= \frac{1}{V_a} \int_{r=a} [q_n] \mathbf{x} \, dS = \mathbf{A}_s^{(12)}(\kappa_1, \kappa_2) \cdot \mathbf{G}, \\ \mathbf{A}_s^{(12)}(\kappa_1, \kappa_2) &= \frac{6\kappa_1^2 C}{\kappa_2 + 2(1+C)\kappa_1} \mathbf{I}, \end{aligned} \quad (4.38)$$

cf. Eq. (2.49).

1.4.3.4 The “Resistive” Spherical Inhomogeneity

The solution of the spherical inhomogeneity problem with a “resisting” interphase is fully similar to the “superconducting” considerations, presented in the previous subsection.

Indeed, the temperature field in this case, before passing to the limit (4.28), has the same form (1.9), (4.29), so that the system (4.30)

for the C_i 's remains the same. When $\delta/a \rightarrow 0$, the unknowns can be expanded as

$$\begin{aligned} C_1 &= C_1^0 + \mathcal{O}\left(\frac{\delta}{a}\right), & C_4 &= C_4^0 + \mathcal{O}\left(\frac{\delta}{a}\right), \\ C_2 &= D \frac{a}{\delta} + C_2^0 + \mathcal{O}\left(\frac{\delta}{a}\right), & C_3 &= -D \frac{a}{\delta} + C_3^0 + \mathcal{O}\left(\frac{\delta}{a}\right), \end{aligned} \quad (4.39)$$

retaining only the terms that matter in the limit (4.28). Taking this limit yields

$$\begin{aligned} C_1^0 &= \frac{3D}{R}, & C_1^0 + 3D &= 1 + C_4^0, \\ \kappa_2 C_1^0 &= \kappa_1(1 - 2C_4^0), & C_1^0 &= C_2^0 + C_3^0, \end{aligned} \quad (4.40)$$

having recalled Eq. (4.32). The constants C_2^0 and C_3^0 remain undefined; they however describe the solution within the disappearingly thin coating. Moreover, only their sum, i.e. C_1^0 , matters, see Eq. (4.40). Solving the system (4.40) is elementary: the single sphere field in the resistance case has again the familiar form (1.14), namely,

$$\theta(\mathbf{x}) = \mathbf{G} \cdot \mathbf{x} \begin{cases} \gamma^r, & \text{if } |\mathbf{x}| < a, \\ 1 - \beta^r (a/r)^3, & \text{if } |\mathbf{x}| > a, \end{cases} \quad (4.41)$$

with the constants

$$\begin{aligned} \gamma^r &= C_1^0 = \frac{3\kappa_1}{\kappa_2 + 2(1+R)\kappa_1}, \\ \beta^r &= -C_4^0 = \frac{\kappa_2 - (1+R)\kappa_1}{\kappa_2 + 2(1+R)\kappa_1}. \end{aligned} \quad (4.42)$$

The temperature field (4.41) jumps at the inclusion surface $r = a$:

$$\begin{aligned} [\theta] \Big|_{r=a} &= \left(\theta^{(1)} - \theta^{(2)} \right) \Big|_{r=a} \\ &= RC_1^0 \mathbf{G} \cdot \mathbf{x} = \frac{3R\kappa_1}{\kappa_2 + 2(1+R)\kappa_1} \mathbf{G} \cdot \mathbf{x}. \end{aligned} \quad (4.43)$$

Hence the interphase concentration factor $\mathbf{B}_s^{(12)}$, for a single sphere

(we again underline this adding the subscript ‘s’), is

$$\begin{aligned}\overline{\Theta}_s^{(12)} &= \frac{1}{V_a} \int_{r=a} [\theta] \mathbf{n} \, dS = \mathbf{B}_s^{(12)}(\kappa_1, \kappa_2) \cdot \mathbf{G}, \\ \mathbf{B}_s^{(12)}(\kappa_1, \kappa_2) &= \frac{3R\kappa_1}{\kappa_2 + 2(1+R)\kappa_1} \mathbf{I},\end{aligned}\tag{4.44}$$

cf. Eq. (2.52).

Note that at $r = a$ the heat flux, being continuous, is proportional to this jump:

$$\kappa_1 \frac{\partial \theta^{(1)}}{\partial r} = \kappa_2 \frac{\partial \theta^{(2)}}{\partial r} = \frac{\kappa_2}{aR} (\theta^{(1)} - \theta^{(2)}) \quad \text{at } r = a.\tag{4.45}$$

The boundary condition (4.45) corresponds to the so-called *skin effect*, and the proportionality coefficient in it, $\kappa_2/(aR)$, is the *skin constant*.¹³ The skin effect reflects the phenomenon, known as *Kapitza’s resistance* of an interphase boundary, see, for example, the papers [BEb], [BEf], [TOd], [MIa] *et al.* and the references therein, as well as the original Kapitza’s work of 1941, translated in [KAh, p. 561]. (This kind of resistance is well pronounced at very low temperatures, increasing dramatically at temperatures $T < 20$ K.) Note also that the more general ellipsoidal inclusion problem for the resistance case, i.e. under the boundary condition (4.45), is much more complicated than that for the ideal contact. The analytical solution is obtained in the paper of Benveniste and Miloh [BEf]; our elementary formula, Eqs. (4.41) and (4.42), for spherical shape is given there as a particular case (cf. their Eq. (82)); the skin constant is denoted in this paper as β (so that $\beta = \kappa_2/(aR)$ in our notations).

Remark 4.4 *It is worth noting that the exact counterpart of the Kapitza resistance in elasticity context is the so-called “Hooke law” for a thin inhomogeneity, spread along the 2-D surface Σ [SOa]. More precisely, for a “crack-like” inclusion, when the stress vector $\boldsymbol{\sigma}_n$ is continuous on Σ , one has*

$$\boldsymbol{\sigma}_n(\mathbf{x}) = \boldsymbol{\lambda}(\mathbf{x}) \cdot [\mathbf{u}(\mathbf{x})], \quad \mathbf{x} \in \Sigma,\tag{4.46}$$

¹³Often the condition (4.45) is associated with the *interfacial thermal barrier resistance*; in composites this effect arises due to poor mechanical or chemical adherence, mismatch of the coefficients of thermal expansions leading to interfacial gaps (microcracks). For more details and references see the papers of Hasselman *et al.* [HAo], [HAp].

which means that the “opening” of the inclusion, $[\mathbf{u}(\mathbf{x})]$, is proportional to the normal stress vector $\boldsymbol{\sigma}_n(\mathbf{x})$ on the surface Σ . The second-rank tensor $\boldsymbol{\lambda}(\mathbf{x})$ in (4.46) is just the “Hooke tensor” for the inclusion, see [SOa], [KAc] for more details and discussion.

1.4.4 Elastic Case

In this case the counterpart of Eq. (4.1) reads

$$\mathbb{L}(\mathbf{x}) = \mathbb{L}_1 + [\mathbb{L}]h_w(\mathbf{x}), \quad [\mathbb{L}] = \mathbb{L}_2 - \mathbb{L}_1, \quad (4.47)$$

where $h_w(\mathbf{x})$ is again the characteristic function of the inhomogeneity \mathcal{W} , \mathbb{L}_1 and \mathbb{L}_2 are the tensors of the elastic moduli of the matrix and of the inhomogeneity, respectively. At the absence of body forces, the displacement field $\mathbf{u}(\mathbf{x})$ in the solid obeys the equation

$$\nabla \cdot \{\mathbb{L}_1 : \nabla \mathbf{u}(\mathbf{x})\} + \nabla \cdot \{h_w(\mathbf{x})[\mathbb{L}] : \nabla \mathbf{u}(\mathbf{x})\} = 0, \quad (4.48)$$

see Eqs. (2.54) and (4.47).

Similarly to the scalar case (Section 1.4.2), the basic integral equation which governs the strain tensor field in the solid with a single inhomogeneity, follows directly from Eq. (4.48). In a Cartesian system it has the form

$$\varepsilon_{in}(\mathbf{x}) = \varepsilon_{in}^\infty(\mathbf{x}) + \int_{\mathcal{W}} \mathbb{G}_{ipjn}(\mathbf{x} - \mathbf{x}') [\mathbb{L}]_{pjkl} \varepsilon_{kl}(\mathbf{x}') d\mathbf{x}', \quad (4.49)$$

where

$$\mathbb{G}_{ipjn}(\mathbf{x}) = \frac{1}{2} (G_{ip,jn}(\mathbf{x}) + G_{np,ji}(\mathbf{x})) \quad (4.50)$$

is the counterpart of the kernel (4.5), with $G_{ij}(\mathbf{x})$ denoting the component of the Green tensor for an unbounded matrix.

For an isotropic matrix the Green tensor is well-known

$$G_{ij}(r) = \frac{1}{4\pi\mu_1} \left(\frac{1}{r} \delta_{ij} + \kappa_1 r_{,ij} \right), \quad \kappa_1 = -\frac{1}{4(1-\nu_1)}, \quad (4.51)$$

$r = |\mathbf{x}|$, where μ_1 and ν_1 are the shear modulus and the Poisson ratio of the matrix.

Let $\varepsilon^\infty = \text{const}$; from Eq. (4.49) it is easily seen that the strain within the inhomogeneity \mathcal{W} will be also constant, if the tensor field

$$\begin{aligned} \mathbb{P}_{ipjn}(\mathbf{x}) &= - \int_{\mathcal{W}} \mathbb{G}_{ipjn}(\mathbf{x} - \mathbf{x}') d\mathbf{x}' \\ &= - \frac{1}{\mu_1} \left[\frac{1}{2} (\varphi_{,jn}(\mathbf{x}) \delta_{ip} + \varphi_{,ji}(\mathbf{x}) \delta_{np}) + \kappa_1 \psi_{,ipjn} \right] \end{aligned} \quad (4.52)$$

is constant within the inhomogeneity \mathcal{W} ; here $\varphi = \varphi_w(\mathbf{x})$ is the Newtonian potential (4.8) and

$$\psi(\mathbf{x}) = \psi_w(\mathbf{x}) = \frac{1}{4\pi} \int_{\mathcal{W}} |\mathbf{x} - \mathbf{x}'| \, d\mathbf{x}' \quad (4.53)$$

is the biharmonic potential for the region \mathcal{W} ; recall that the latter solves the equations

$$\Delta\psi_w(\mathbf{x}) = 2\varphi_w(\mathbf{x}), \quad \Delta\Delta\psi_w(\mathbf{x}) + 2h_w(\mathbf{x}) = 0. \quad (4.54)$$

In turn, \mathbb{P} will be constant within \mathcal{W} , if $\varphi_w(\mathbf{x})$ is a quadratic function and $\psi_w(\mathbf{x})$ is a polynomial of fourth degree there. The latter is again true for an ellipsoidal inhomogeneity. We can thus conclude, similarly to the scalar case, that if the strain tensor at infinity is constant, it will be also constant within any such inhomogeneity, see e.g. [ESa], [KUb], [CHd], etc. Moreover, as it follows from Eq. (4.49),

$$\mathbb{A}_w = \left(\mathbb{I} + \mathbb{P} : [\mathbb{L}] \right)^{-1}, \quad (4.55)$$

where \mathbb{I} is the “unit” fourth rank tensor with the Cartesian components $\mathbb{I}_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$.

The tensor \mathbb{A}_w in Eq. (4.55), that interconnects the constant strain at infinity with the constant strain in the ellipsoid, is often called in the literature *Wu*'s. (Wu was the first who specified this tensor for a spheroid, averaged over all possible orientations, and then treated the limiting cases of a disk and fiber in order to clarify the influence of the shape upon the effective elastic properties [WUa].)

Remark 4.5 *Note, without going into details, that once the strain tensor within the inclusion is found, i.e. the tensor \mathbb{A}_w is specified, the displacement and strain fields outside the inclusion can be immediately obtained by means of the basic integral equation (4.49), cf. Remark 4.3, where the similar question was discussed in the scalar case.*

Consider first, similarly to the scalar case, the most important particular shapes of the inclusion \mathcal{W} .

- Let the inhomogeneity \mathcal{W} be a *sphere*. Both tensors $\nabla\nabla\varphi_w(\mathbf{x})$ and $\nabla\nabla\nabla\nabla\psi_w(\mathbf{x})$ are then constant and isotropic, if $\mathbf{x} \in \mathcal{W}$; $\nabla\nabla\varphi_w(\mathbf{x})$ is given in Eq. (4.11) and

$$\psi_{,ijkl} = \alpha\mathbb{H}_{ijkl}, \quad \mathbb{H}_{ijkl} = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}, \quad \mathbf{x} \in \mathcal{W}, \quad (4.56)$$

since ψ_{ijkl} should be completely symmetric with respect to its indices. Making a full contraction in (4.56) and utilizing Eq. (4.54)₂, we find $\alpha = -2/15$, so that

$$\nabla\nabla\nabla\nabla\psi_w(\mathbf{x}) = -\frac{2}{15}\mathbb{H}, \quad \mathbf{x} \in \mathcal{W}. \quad (4.57)$$

Eqs. (4.11), (4.57) and (4.52) now specify the needed tensor \mathbb{A}_w :

$$\begin{aligned} \mathbb{A}_w &= \frac{k_1}{k_1 + \alpha_1[k]} \mathbb{I}' + \frac{\mu_1}{\mu_1 + \beta_1[\mu]} \mathbb{I}'' \quad (\text{sphere}), \\ \mathbb{I}'_{ijkl} &= \frac{1}{3}\delta_{ij}\delta_{kl}, \quad \mathbb{I}''_{ijkl} = \frac{1}{2} \left(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right), \\ \alpha_1 &= \frac{3k_1}{3k_1 + 4\mu_1} = \frac{1 + \nu_1}{3(1 - \nu_1)}, \\ \beta_1 &= \frac{6}{5} \frac{k_1 + 2\mu_1}{3k_1 + 4\mu_1} = \frac{2}{15} \frac{4 - 5\nu_1}{1 - \nu_1}, \end{aligned} \quad (4.58)$$

with $k_1 = \lambda_1 + \frac{2}{3}\mu_1$ denoting the bulk modulus of the matrix.

• Let the inhomogeneity \mathcal{W} represent a *circular fiber* along the axis x_3 . The second gradient $\nabla\nabla\varphi_w$ in this case has been found in Eq. (4.14). We introduce the 2-D counterparts $\mathbb{D} = \|\mathbb{D}_{ijkl}\|$ of the fully symmetric tensor \mathbb{H} from Eq. (4.56), $i, j = 1, 2$. Then $\psi_{ijkl} = \alpha\mathbb{D}_{ijkl}$; using Eqs. (4.54) and (4.53) gives $\alpha = -1/4$ and hence

$$\nabla\nabla\nabla\nabla\psi_w = -\frac{1}{4}\mathbb{D}. \quad (4.59)$$

Let us recall the short-hand notation of Hill [HIId]. If a pair of symmetric second-rank tensors $\mathbf{\Sigma}$, \mathbf{T} with the Cartesian components $\|s_{ij}\|$ and $\|t_{ij}\|$, respectively, are interrelated in the same Cartesian system as

$$\begin{aligned} \frac{1}{2}(s_{11} + s_{12}) &= a(t_{11} + t_{12}) + b't_{33}, \\ s_{33} &= b''(t_{11} + t_{12}) + ct_{33}, \quad s_{11} - s_{12} = 2d(t_{11} - t_{22}), \\ s_{12} &= 2dt_{12}, \quad s_{13} = 2et_{13}, \quad s_{23} = 2et_{23}, \end{aligned} \quad (4.60)$$

then the transversely isotropic fourth-rank tensor \mathbb{A} (with the symmetry axis x_3), such that $\mathbf{\Sigma} = \mathbb{A} : \mathbf{T}$, is symbolically written as

$$\mathbb{A} = (2a, b', b'', c, 2d, 2e). \quad (4.61)$$

Using these notations and the already found gradients of the potentials φ_w and ψ_w , see Eq. (4.59), we have eventually

$$\begin{aligned} \mathbb{A}_w &= (2A, B', B'', C, 2D, 2E) \quad (\text{fiber}), \\ 2A &= \frac{\lambda_1 + 2\mu_1}{\lambda_2 + \mu_2 + \mu_1}, \quad 2B' = -\frac{[\lambda]}{\lambda_2 + \mu_2 + \mu_1}, \\ B'' &= 0, \quad C = 1, \quad 2D = \frac{4(1 - \nu_1)}{1 + (3 - 4\nu_1)g}, \\ 2E &= \frac{2\mu_1}{\mu_2 + \mu_1}, \quad g = \frac{\mu_2}{\mu_1}, \quad [\lambda] = \lambda_2 - \lambda_1. \end{aligned} \tag{4.62}$$

• Let the inhomogeneity be a *layer* $-h \leq x_3 \leq h$, perpendicular to the x_3 -axis. The potential φ and ψ will then depend on x_3 solely and utilizing once again simple symmetry arguments yields

$$\varphi_{ij} = -\delta_{3i}\delta_{3j}, \quad \psi_{ijkl} = -2\delta_{3i}\delta_{3j}\delta_{3k}\delta_{3l}.$$

These expressions, together with Eqs. (4.55) and (4.52), give eventually

$$\begin{aligned} \mathbb{A}_w &= (2A, B', B'', C, 2D, 2E) \quad (\text{layer}), \\ 2A &= 1, \quad B' = 0, \quad B'' = -\frac{[\lambda]}{\lambda_2 + 2\mu_2}, \\ C' &= \frac{\lambda_1 + 2\mu_1}{\lambda_2 + 2\mu_2}, \quad 2D = 1, \quad 2E = \frac{\mu_1}{\mu_2}. \end{aligned} \tag{4.63}$$

• Consider next the more general case of a *spheroidal inhomogeneity* \mathcal{W} . The needed second gradient of the Newtonian potential is given in Eq. (4.20). In turn, using Hill's notations (4.60) and (4.61), and appropriate results, listed in the books of Mura [MUa] or Muratov [MUb], we have, for $\mathbf{x} \in \mathcal{W}$,

$$\begin{aligned} \nabla\nabla\nabla\nabla\psi_w(\mathbf{x}) &= -(4C', C'', C''', 3D', 2C', 2C''), \\ C' &= \frac{1}{4}(1 - 2M) + \frac{3}{8}D', \quad C'' = M - \frac{3}{2}D', \\ D' &= \begin{cases} -\frac{1 - 3M}{3e^2}, & \text{if } c < a, \\ (1 - e^2)\frac{1 - 3M}{3e^2}, & \text{if } c > a, \end{cases} \end{aligned} \tag{4.64}$$

where M , M_\perp , ξ and the eccentricity e , let us recall, are defined in Eq. (4.20).

In the isotropic case under study it remains to introduce Eqs. (4.20) and (4.64) into Eq. (4.55) in order to find the needed fourth-rank tensor \mathbb{A}_w that transforms the strain in infinity into the strain within the spheroidal inhomogeneity. After some algebra, the eventual result reads

$$\begin{aligned} \mathbb{A}_w &= (2A, B', B'', C, 2D, 2E) \quad (\text{spheroid}), \\ 2A &= \frac{1}{2\Lambda} \left\{ 1 + \frac{1}{\gamma_1} \left(M[\gamma] + 2\chi_1 C''[\mu] \right) \right\}, \\ 2B' &= -\frac{1}{\Lambda\gamma_1} \left\{ M_\perp[\lambda] - \chi_1 C''[\mu] \right\}, \\ 2B'' &= l - \frac{1}{\Lambda\gamma_1} \left\{ M[\lambda] - \chi_1 C''[\mu] \right\}, \\ C &= \frac{1}{2\Lambda} \left\{ 1 + \frac{1}{\gamma_1} \left(2M_\perp[\lambda] + ([\mu] + \chi_1 C'')[\mu] \right) \right\}, \\ 2D &= \frac{\mu_1}{\mu_1 + 2(M_\perp + 2\kappa_1 C')[\mu]}, \\ 2E &= \frac{\mu_1}{\mu_1 + (M + M_\perp + 4\kappa_1 C'')[\mu]}, \\ 2\Lambda &= 1 + \frac{1}{\gamma_1} \left\{ [k] + \left(3\chi_1 C'' + M + \frac{1}{3} \right) [\mu] \right\} \\ &+ \frac{3}{\gamma_1^2} \left(\chi_1 C'' + 2MM_\perp \right) [k][\mu], \quad \chi_1 = \frac{\lambda_1 + \mu_1}{\mu_1} = \frac{1}{1 - 2\nu_1}, \end{aligned} \quad (4.65)$$

$$\gamma_i = \lambda_i + 2\mu_i, \quad i = 1, 2.$$

Remark 4.6 *Once again, for the particular values of the parameters M_\perp and M , as listed in Eq. (4.22), the particular forms of the tensor \mathbb{A}_w are recovered from (4.65) for a sphere, fiber and layer, cf. Eqs. (4.58), (4.62) and (4.63), respectively.*

• Let the spheroid be randomly (and uniformly) oriented in the space. Then

$$\langle \mathbb{A}_w \rangle_\Omega = a' \mathbb{I}' + a'' \mathbb{I}'', \quad (4.66)$$

where $\langle \mathbb{A}_w \rangle_\Omega$ denotes the value of the tensor \mathbb{A}_w averaged with respect to all possible orientations of the axes x_i of the spheroid; the isotropic

tensors \mathbb{I}' and \mathbb{I}'' are defined in Eq. (4.58). After some algebra, it appears eventually

$$\begin{aligned} a' &= \frac{1}{3}(4A + 2B' + 2B'' + C) \\ &= \frac{1}{2\Lambda} \left\{ 1 + \frac{1}{\gamma_1} \left(M + \frac{1}{3} + 3\chi_1 C''[\mu] \right) \right\}, \\ a'' &= \frac{1}{15} (2A - 2B' - 2B'' + 2C + 12D + 12E). \end{aligned} \quad (4.67)$$

Unlike a' , we were not able to find a simpler expression for the coefficient a'' .

The quantities a' and a'' have been first calculated by Wu [WUa], and also by Kuster and Toksöz [KUC], some misprints are corrected in [BEm]. A simple check shows that though different functions are used (e.g. $\operatorname{arcsinh} \xi$), the basic parameter θ , used in the papers [WUa], [BEm] is simply $1 - M$, where M is the depolarization factor from Eq. (4.20).

• *The “Crack” Limit.* In Section 1.5, when dealing with the effective properties of microcracked solids, we shall need information about the asymptotic behavior of the tensor \mathbb{A}_w , given in Eq. (4.65), when the ratio $\xi = c/a \rightarrow 0$. The reason is that the cracks will be treated as degenerating spheroids, in the sense that while two of the axes $a = b$ are kept fixed, the third one, c , becomes negligibly small, i.e. $c/a \rightarrow 0$. From the definitions of the respective parameters, see Eqs. (4.20) and (4.65), it is easily checked that the following formulae hold as $\xi \rightarrow 0$, namely,

$$\begin{aligned} M &= 1 - \frac{\pi}{2}\xi + \mathcal{O}(\xi), \quad M_{\perp} = \frac{\pi}{4}\xi + \mathcal{O}(\xi), \quad C' = 0.0625\pi\xi + \mathcal{O}(\xi), \\ C'' &= \frac{\pi}{4}\xi + \mathcal{O}(\xi), \quad D' = \frac{2}{3} - \frac{\pi}{2}\xi + \mathcal{O}(\xi), \quad \gamma = \frac{2}{3\pi} \frac{1}{\xi} + \mathcal{O}(1), \\ \Lambda &= \Lambda_0\xi + \mathcal{O}(\xi), \quad \Lambda_0 = \frac{\pi}{8} \frac{1 - 2\nu_1}{(1 - 2\nu_1)^2}, \\ A &= \frac{1}{4} \frac{1 - 2\nu_1}{1 - 2\nu_1} \frac{1}{\xi} + \mathcal{O}(1), \quad B' = -\frac{1}{4}(1 - \nu_1) + \mathcal{O}(\xi), \\ C &= \frac{4}{\pi} \frac{1 - 2\nu_1}{1 - 2\nu_1} \frac{1}{\xi} + \mathcal{O}(1), \quad B'' = \frac{4}{\pi} \frac{\nu_1(1 - \nu_1)}{1 - 2\nu_1} \frac{1}{\xi} + \mathcal{O}(1), \end{aligned} \quad (4.68)$$

$$\begin{aligned}
D &= \frac{1}{2} + \pi\xi \left(1 - \frac{0.0125}{1 - \nu_1}\right) + o(\xi), & E &= \frac{2}{\pi} \frac{1 - \nu_1}{2 - \nu_1} \frac{1}{\xi} + \mathcal{O}(1), \\
a' &= \frac{1}{3}(4A + 2B' + 2B'' + C) = \frac{4}{3\pi} \frac{1 - \nu_1^2}{1 - 2\nu_1} \frac{1}{\xi} + \mathcal{O}(1), \\
a'' &= \frac{1}{15}(2A - 2B' - 2B'' + 2C + 12D + 12E) \\
&= \frac{8}{15\pi} \frac{(1 - 2\nu_1)(5 - \nu_1)}{2 - \nu_1} \frac{1}{\xi} + \mathcal{O}(1).
\end{aligned}$$

1.5 One-Particle Approximations

For simplicity, we shall consider the so-called *particulate media*, in which one of the constituents, called *matrix*, is connected. Throughout the latter particles of a second constituent (*filler*), with a well-defined, in general, shapes are distributed. The properties of the matrix and of the filler are denoted, similarly to the previous section, by ‘1’ and ‘2’, respectively, so that, e.g. κ_1 and κ_2 are the appropriate conductivities, etc. Such a material is called also a *dispersion* (to be thus distinguished from the case of suspension, when the particles are immersed into a liquid and hence their relative positions are not fixed due to the flow—a fact that tremendously complicates any theoretical study).

Our aim here will be to demonstrate how various “repetitions” (to cite again Maxwell [MAj, Section 314]) of the single-inclusion solutions of Section 1.1.3.3 can be systematically utilized in order to derive the basic and most widely used approximate models for predicting the effective properties of particulate media.

The basic idea is to invoke formulae like (2.41) that interconnect the effective properties with the appropriate concentration factors, as introduced in Sections 1.2.6—1.2.8. The latter are in turn *approximated* by the appropriate solutions of the single-inclusion problem.

Two natural possibilities are then opened. They can be summarized as follows:

- (i) *Each inclusion is treated as single, immersed into a homogeneous medium. The latter, as a consequence of the presence*

of the host of other inclusions, possesses the unknown effective properties (the effective medium idea).

- (ii) Each inclusion is again treated as single, but now immersed into the matrix. The presence of the rest of inclusions is accounted for by imagining that the inclusion is subjected to a certain external field that differs from the applied macroscopic one (the effective field idea).

We shall consider below some of the simplest implementations of the assumptions (i) and (ii), within the frame of the static behavior of heterogeneous media. Their application and generalization for wave propagation problems in such media are discussed and treated in detail in Chapter 3 of this volume.

1.5.1 Dilute Filler Fraction—Scalar Conductivity

Let us start with the simplest case, when there is no need either to modify the medium's properties or to change the applied field.

Namely, let the dispersion contain identical particles, of a fixed shape \mathcal{W} , aligned throughout the matrix. We assume that the dispersion is *dilute*, in the sense that the volume fraction, ϕ_2 , of the particles is small, $\phi_2 \ll 1$, and hence their mutual influence can be neglected. Each particle can be thus imagined as *single*, immersed into an unbounded matrix, and the “concentration factor” \mathbf{A}_2 is simply the single-inhomogeneity tensor $\mathbf{A}_w(\kappa_1, \kappa_2)$, defined in Eq. (4.10). Thus, as it follows from (2.41),

$$\mathbf{K}^* = \kappa_1 \mathbf{I} + \phi_2 [\kappa] \mathbf{A}_w(\kappa_1, \kappa_2) + \mathcal{O}(\phi_2) \quad (5.1)$$

—both constituents are assumed isotropic but, due to the alignment and nonspherical, in general, shape of the particles, the effective tensor \mathbf{K}^* may be anisotropic. As underlined in (5.1), the formula is correct to the order $\mathcal{O}(\phi_2)$ only, providing however in this case an *exact* expression (since the particle interactions are *totally* neglected). To get the successive terms of order ϕ_2^2 and higher, these interactions should be somehow accounted for. But, naturally, all schemes considered below, that try to incorporate the interactions, agree in the dilute limit. More precisely, they all reproduce the formula (5.1) in this case.

Remark 5.1 Note that the approximation (5.1) has been used in many of the earlier works on conductivity of two-phase media also in the non-dilute case, see [REb] for some references. Perhaps its origin can be traced back to Laplace himself: According to Lorentz' [LOb, Section 123], considering the connection between the density, ρ , of a transparent solid and its refraction index, μ^2 , Laplace reached the formula

$$\frac{\mu^2 - 1}{\rho} = \text{const.} \quad (5.2)$$

But μ^2 is just the dielectric constant of the medium, as already pointed out (see the footnote on page 10), and the density ρ is proportional to the volume fraction of the dielectric spheres contained in the medium. Then (5.2) can be interpreted, somewhat loosely of course, as the dilute approximation of the type (5.1) for the effective dielectric constant of a dispersion.

Remark 5.2 “Dilute” formulae like (5.1) can be derived for heterogeneous media in different physical context (see, e.g. Section 1.5.7 below where the absorption problem is addressed). The so-obtained results will make sense, however, only if the solution of the appropriate single-inclusion problem exists and is finite, like the tensor \mathbf{A}_w in Eq. (5.1). There are, unfortunately, situations when this solution does not exist (say, for the same absorption problem in 2-D, see again the same Section 1.5.7). Then the appropriate effective properties have no representation of the type (5.1); nonanalytic functions, like $\ln \phi_2$, may emerge for small $\phi_2 \ll 1$ instead.

Consider in more detail the most important particular cases of the formula (5.1).

- Assume the inhomogeneities are *spheres*. From Eqs. (4.13) and (5.1) it follows

$$\frac{\kappa^*}{\kappa_1} = 1 + 3\beta\phi_2 + \mathcal{O}(\phi_2^2), \quad \beta = \frac{[\kappa]}{\kappa_1 + 2\kappa_2}, \quad (5.3)$$

which, naturally enough, reproduces the dilute limit (1.20) of the Maxwell prescription for κ^* .

- Consider a *fiber-reinforced material*, in which inhomogeneities are parallel circular cylinders (along the axis x_3). The effective

conductivity tensor is transversely isotropic

$$\mathbf{K}^* = \kappa_{11}^*(\mathbf{e}_1\mathbf{e}_1 + \mathbf{e}_2\mathbf{e}_2) + \kappa_{33}^*\mathbf{e}_3\mathbf{e}_3, \quad (5.4)$$

where

$$\kappa_{11}^* = \kappa_{22}^* = \kappa_1 \left(1 + \frac{2[\kappa]}{\kappa_1 + \kappa_2} \phi_2 \right) + \mathcal{O}(\phi_2), \quad (5.5)$$

$$\kappa_{33}^* = \bar{\kappa} = \phi_1\kappa_1 + \phi_2\kappa_2,$$

see (5.1) and (4.15). The coefficients $\kappa_{11}^* = \kappa_{22}^*$ represent the transverse conductivity of the fiber-reinforced medium, for dilute fiber concentration $\phi_2 \ll 1$, in the case when the applied temperature gradient is perpendicular to fibers' axes. The conductivity component κ_{33}^* along the x_3 -axis is *exactly* the arithmetic mean $\bar{\kappa}$, which explains why the higher order correction $\mathcal{O}(\phi_2)$ is missing in the second formula of (5.5). The reason is that the temperature field in the medium is just $\theta(\mathbf{x}) \equiv G_3x_3$, if the applied gradient is along the fibers, i.e. if $\mathbf{G} = G_3\mathbf{e}_3$ —a situation already discussed in Remark 2.1, see Eq. (2.11).

- Consider a *layered material* that consists of laminae, perpendicular to the axis x_3 . The appropriate tensor \mathbf{A}_w is given in (4.17), so that Eq. (5.1) implies

$$\kappa_{11}^* = \kappa_{22}^* = \kappa_1 + \phi_2[\kappa] + \mathcal{O}(\phi_2), \quad \kappa_{33}^* = \kappa_1 + \phi_2[\kappa] \frac{\kappa_1}{\kappa_2} + \mathcal{O}(\phi_2).$$

However, for such an exceptionally simple internal constitution the following *exact* formulae for the effective conductivities hold

$$\kappa_{11}^* = \kappa_{22}^* = \bar{\kappa}, \quad \text{i.e.} \quad 1/\kappa^* = \overline{1/\kappa} = \phi_1/\kappa_1 + \phi_2/\kappa_2. \quad (5.6)$$

The reason is that the temperature gradient remains constant within the volume \mathcal{V} , if \mathbf{G} is along the laminae. If \mathbf{G} is along the axis x_3 , i.e. perpendicular to the laminae, the heat flux is constant within \mathcal{V} ; in this case the effective compliance $k^* = 1/\kappa^*$ is the arithmetic mean of the constituents' compliances, see Remark 2.2 and Eq. (2.18).

- Let the inhomogeneities be *identical and isotropic spheroids*, aligned along the x_3 -axis, with the semiaxes c and a , $c \neq a = b$. In this case the tensor \mathbf{A}_w is given in Eq. (4.21), the medium is

transversely isotropic, with symmetry axis x_3 , and its effective conductivity tensor \mathbf{K}^* is

$$\begin{aligned}\mathbf{K}^* &= \kappa_{11}^* (\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) + \kappa_{33}^* \mathbf{e}_3 \mathbf{e}_3, \\ \kappa_{11}^* &= \kappa_{22}^* = \kappa_1 \left(1 + \phi_2 \frac{[\kappa]}{\kappa_1 + [\kappa] M_\perp} \right) + \mathcal{O}(\phi_2), \\ \kappa_{33}^* &= \kappa_1 \left(1 + \phi_2 \frac{[\kappa]}{\kappa_1 + [\kappa] M} \right) + \mathcal{O}(\phi_2).\end{aligned}\quad (5.7)$$

For the particular values of the parameters M and M_\perp , as listed in Eq. (4.22), the already given formulae (5.3), (5.5) and (5.6) for the effective conductivities in the cases of spheres, fibers and layers, respectively, show up.

- Let the inhomogeneities be again identical, but *randomly oriented and isotropic spheroids*, with the semiaxes c and a . In this case the tensor $\mathbf{A}_w = \langle \mathbf{A}_w \rangle_\Omega$ is given in Eq. (4.23), the medium is macroscopically isotropic and its effective conductivity reads

$$\frac{\kappa^*}{\kappa_1} = 1 + \frac{[\kappa]}{3\kappa_1} \left(\frac{2\kappa_1}{\kappa_1 + [\kappa] M_\perp} + \frac{\kappa_1}{\kappa_1 + [\kappa] M} \right) \phi_2 + \mathcal{O}(\phi_2). \quad (5.8)$$

The parameters M and M_\perp depend on the eccentricity of the spheroids, see Eq. (4.20).

- Let the spheroids, again randomly oriented in the space, degenerate into *penny-shaped cracks*. In this case $\kappa_2 = 0$ and the term in the brackets in the right-hand side of (5.8) has the asymptotic

$$m = \frac{2}{1 - M_\perp} + \frac{1}{1 - M} = \frac{2}{\pi} \frac{1}{\xi} + \mathcal{O}(\xi), \quad \xi = c/a \rightarrow 0, \quad (5.9)$$

as it follows from Eq. (4.68). Eq. (5.8) now yields

$$\begin{aligned}\frac{\kappa^*}{\kappa_1} &= 1 - n \frac{4}{3} \pi a^2 c m = 1 - (na^3) \frac{4}{3} \pi \frac{c}{a} m \\ &= 1 - \varepsilon \frac{4}{3} \pi \xi m + \mathcal{O}(\xi) \xrightarrow{\xi \rightarrow 0} 1 - \frac{8}{9} \varepsilon,\end{aligned}\quad (5.10)$$

in virtue of Eq. (5.9). Here n is number density of the spheroids (i.e. their number per unit volume), so that $\phi_2 = nV$, $V = \frac{4}{3} \pi a^2 c$ is the volume of the single spheroid, and

$$\varepsilon = na^3 \quad (5.11)$$

is the so-called *crack density parameter*—the counterpart of the volume fraction of the inclusions in the case of cracked solids (as introduced and very often employed for such solids, see the survey of Kachanov [KAa]). Thus the effective conductivity of a solid, containing a dilute population of randomly oriented penny-shaped cracks, is

$$\frac{\kappa^*}{\kappa_1} = 1 - \frac{8}{9}\varepsilon + \mathcal{O}(\varepsilon), \quad (5.12)$$

1.5.2 Dilute Filler Fraction—Elastic Case

In the elastic case and for a dilute particle concentration we have, as a consequence of Eq. (2.64),

$$\mathbb{L}^* = \mathbb{L}_1 + \phi_2[\mathbb{L}] : \mathbb{A}_w(\mathbb{L}_1, \mathbb{L}_2) + \mathcal{O}(\phi_2), \quad (5.13)$$

where \mathbb{A}_w is the fourth-rank tensor that comes out from the solution of the elastic single inclusion problem, see Section 1.4.4.

Remark 5.3 *Since the formula (5.13) is exact, the tensor*

$$[\mathbb{L}] : \mathbb{A}_w(\mathbb{L}_1, \mathbb{L}_2)$$

possesses the needed “external” symmetry (2.65), whatever the shape of the inclusions \mathcal{W} .

Similarly to the previous subsection, consider the most interesting particular cases of the formula (5.13).

- For an *isotropic dispersion of spheres* the tensor \mathbb{A}_w is given in Eq. (4.58) and hence

$$\begin{aligned} \frac{k^*}{k_1} &= 1 + \frac{[k]}{k_1 + \alpha_1[k]} \phi_2 + \mathcal{O}(\phi_2), \\ \frac{\mu^*}{\mu_1} &= 1 + \frac{[\mu]}{\mu_1 + \beta_1[\mu]} \phi_2 + \mathcal{O}(\phi_2); \end{aligned} \quad (5.14)$$

α_1 and β_1 depend on the Poisson ratio, ν_1 , of the matrix, see the same Eq. (4.58).

Remark 5.4 *The formulae (5.14) have been first derived by Bruggerman [BRg]. (Though, as pointed out in [ESa], his result for the shear*

modulus is apparently incorrect, since the Poisson ratio of the matrix does not appear.) The correct formula for μ^* was given by Dewey [DEb]. The particular case of (5.14) for rigid particles was found by Hashin [HAc]. Eshelby [ESa] obtained them as a consequence of his well-known solution for the ellipsoidal inhomogeneity problem. Hashin [HAD] rederived independently the same formulae and, on their base, proposed a method how the nondilute case could be treated. In the wave propagation problem for a dilute dispersion, the same formula (5.14) reappeared as a zero-frequency limit [CHa], [MAb]. (In the Russian literature Eqs. (5.14) are often attributed to Krivoglaz and Cherevko [KRc].) As it seems, Eqs. (5.14) are one of the most often rederived formulae in the elasticity of two-phase media for a period at least of forty years (1937–1957); the author suspects that the foregoing list of references is far from exhaustive.

Remark 5.5 For a porous solid ($k_2 = \mu_2 = 0$), the formulae (5.14) simplify

$$\begin{aligned}\frac{k^*}{k_1} &= 1 - \frac{3}{2} \frac{1 - \nu_1}{1 - 2\nu_1} \phi_2 + \mathcal{O}(\phi_2), \\ \frac{\mu^*}{\mu_1} &= 1 - 15 \frac{1 - \nu_1}{7 - 5\nu_1} \phi_2 + \mathcal{O}(\phi_2)\end{aligned}\tag{5.15}$$

—in this case they are due to Mackenzie [MAa].

Remark 5.6 Let the matrix be incompressible, so that $k_1 = \infty$, $\nu_1 = 0.5$, and the spherical particles are rigid, $k_2 = \mu_2 = \infty$. The shear modulus of such a mixture is then

$$\frac{\mu^*}{\mu_1} = 1 + 2.5\phi_2 + \mathcal{O}(\phi_2),$$

which is exactly the Einstein formula (1.21) for the viscosity of a dilute dispersion. (Observe the full mathematical analogy between the slow (Stokesian) flow of the dispersion, with fixed position of the rigid particles, and the elastic deformation of a solid with the same particles distribution, provided both fluid and solid are incompressible.) In the other limiting case of voids in an incompressible matrix, the second of Eqs. (5.15) yields

$$\frac{\mu^*}{\mu_1} = 1 - \frac{5}{3} \phi_2 + \mathcal{O}(\phi_2).$$

—the counterpart of the Einstein’ formula, giving the viscosity of a dilute bubbly liquid in the Stokesian approximation. This result is attributed to Taylor [TAd].

- Let the inhomogeneities be identical but *randomly oriented spheroids*. Then the material is macroscopically isotropic and (5.13) implies

$$\frac{k^*}{k_1} = 1 + \frac{[k]}{k_1} a' \phi_2 + \mathcal{O}(\phi_2), \quad \frac{\mu^*}{\mu_1} = 1 + \frac{[\mu]}{\mu_1} a'' \phi_2 + \mathcal{O}(\phi_2), \quad (5.16)$$

with the coefficients a' and a'' , given in Eq. (4.67).

- Let $\kappa_2 = 0$ and the spheroids, again randomly oriented in the space, degenerate into *penny-shaped cracks*. Using the asymptotic (4.68) of the coefficients a' and a'' in the “crack” limit, together with Eq. (5.16), one gets

$$\begin{aligned} \frac{k^*}{k_1} &= 1 - \frac{16}{9} \frac{1 - \nu_1^2}{1 - 2\nu_1} \varepsilon + \mathcal{O}(\varepsilon), \\ \frac{\mu^*}{\mu_1} &= 1 - \frac{32}{45} \frac{(1 - \nu_1)(5 - \nu_1)}{2 - \nu_1} \varepsilon + \mathcal{O}(\varepsilon), \end{aligned} \quad (5.17)$$

having recalled the definition (5.11) of the crack density parameter ε .

The formulae (5.17) have been independently proposed by Bristow [BRc] and Walsh [WAa].

Remark 5.7 *Treating the crack as a vacuous oblate spheroid of eccentricity approaching zero is very convenient. To the best of the author’s knowledge it was first employed by Willis [WIb]. The reason is that it allows one to derive straightforwardly the needed formula for a microcracked solid, passing (with a due care) to the appropriate limits in the general formulae, concerning ellipsoidal inclusions. The usefulness of this idea was already demonstrated in deriving Eqs. (5.12) and (5.17). In the elastic context alternative derivations employ specific notions and results from fracture mechanics, like stress-concentration factors, energy release rate, etc. Such a derivation, employed in particular in the original Bristow’s paper [BRc], or in [BEc], is often difficult for a “fracture outsider” to follow.*

1.5.3 Self-Consistent Scheme

When the volume fraction becomes higher (say, $\phi_2 \geq 0.05$) it is not already realistic to imagine the inclusions isolated. Somehow their mutual interactions should be accounted for. The simplest way to do this, at least qualitatively, is the application of the *self-consistent* idea that appeared, in a certain form, already in the Clausius derivation [CLa] of the Maxwell formula, mentioned in Section 1.1. Next it showed up as a very useful and natural tool in solid-state physics and, more specifically, in the wave mechanics of atoms, as originated by Hartree [HAb]. In the context of effective properties of heterogeneous media the self-consistent approach seems to be first employed by Bruggeman [BRf], [BRg], see also [FRd], [LAb]. In the quest of the elastic constants of polycrystals, the method is attributed to Hershey [HEb] and Kröner [KRd]. (In Section 1.6 below we shall present in more details the reasoning and some results of these two authors.)

1.5.3.1 The Basic Idea

The basic idea of the self-consistent scheme (SCS) is to treat each particle again as isolated, but immersed into a matrix possessing the unknown effective properties of the composite. This means that we should replace Eq. (5.1) and its elastic counterpart (5.13) by the equations

$$\begin{aligned} \mathbf{K}^* &= \kappa_1 \mathbf{I} + \phi_2 [\kappa] \mathbf{A}_w(\kappa_1, \mathbf{K}^*) \quad (\text{scalar case}), \\ \mathbb{L}^* &= \mathbb{L}_1 + \phi_2 [\mathbb{L}] : \mathbb{A}_w(\mathbb{L}_1, \mathbb{L}^*) \quad (\text{elastic case}). \end{aligned} \quad (5.18)$$

In each particular case, Eqs. (5.18) will yield appropriate algebraic equations for the unknown effective properties of the composite.

To demonstrate this, consider the simplest example when the inclusions are spheres. In the scalar context, Eq. (4.13) is to be introduced into the first equation of (5.18):

$$\frac{\kappa^*}{\kappa_1} = 1 + \frac{[\kappa]}{\kappa_1} \frac{3\kappa^*}{\kappa_2 + 2\kappa^*} \phi_2 \quad (5.19)$$

which represents, obviously, a quadratic equation with respect to the effective conductivity.

Eq. (5.19) was proposed by Bruggeman [BRf], see also [LAb], in the equivalent form

$$\phi_1 \frac{\kappa_1 - \kappa^*}{\kappa_1 + 2\kappa^*} + \phi_2 \frac{\kappa_2 - \kappa^*}{\kappa_2 + 2\kappa^*} = 0. \quad (5.20)$$

Note the symmetry of the latter with respect to the constituents' characteristics, that is under the simultaneous interchange $\kappa_1 \leftrightarrow \kappa_2$ and $\phi_1 \leftrightarrow \phi_2$. That is why Eq. (5.19) is often called *symmetric effective medium approximation (EMA)*, or First Bruggeman's symmetric EMA—a term, introduced by Landauer [LAc]. Thus each phase should be treated on the same footing, as pointed out by Davies [DAb]; in the above reasoning however one of the phase was imagined continuous, and the second in the form of distributed inclusions; this already implies an inherent logical inconsistency of the SCS. More fundamental, however, is the inconsistency, very clearly exposed by Hashin [HAi], namely, the violation of the basic MMM principle, formulated in Section 1.2.1. The point is that a single sphere in the dispersion is the basic *micro* element and as such it can only “see” the other spheres (micro-elements) around, but *not* the mini-element (the homogenized medium) as a whole, whose properties result from averaging over the multitude of *all* the micro-elements within it. Or, as Hashin put it: *SCS assumes that a tree sees the forest—but a tree sees only other trees.*

The foregoing *does not imply* however that the SCS is useless and should be rejected. It simply suggests that if the scheme is realistic, the appropriate two-phase geometries cannot resemble a dispersion of equi-sized spheres. That this is indeed the case follows from an important result of Milton [MIe]. It states that the SCS (more precisely, Eq. (5.19) or Eq. (5.20)) is a *realizable* approximation in the sense that there exists a special, ingeniously devised, internal geometry of a two-phase medium whose effective elastic moduli coincide *exactly* with the SCS predictions of Eq. (5.19). The reader is referred to the original Milton's work since the details and proofs cannot be elementary summarized. We can only add that, like Hashin's assemblage (Section 1.3.4), the “SCS-geometry” of Milton is of fractal-type (self-similar in all length-scales, that is), comprising inclusions of all possible sizes, from finite down to infinitesimally small. Due to the foregoing remarks, it is a little wonder that such a geometry has nothing in common with equi-sized particles like spheres, distributed throughout a matrix.

Remark 5.8 *The choice of the basic element, to be inserted into the effective medium, is not unique in the SC scheme. In the foregoing, the simplest possibility was chosen, when this is just the filler parti-*

cle. This is however not the only choice; more complicated elements can be devised as well. For example one can take a “composite” sphere, with a kernel of phase ‘1’, coated by a layer of phase ‘2’, as first suggested by Kerner [KEa]. A detailed and critical analysis of such a SCS modification can be found in [HAg]; for generalizations in the elastic case, see [CHe] or [CHd, Chapter 2.3]. This kind of modification of the self-consistent method are usually referred to as Generalized Self-Consistent-Schemes (GSCS), but their discussion goes beyond the frame of the present survey. It should be only noted that without detailed morphological information, no theoretical arguments can be given for any specific choice of a basic element in a binary medium. (The “composite” sphere was used in [CHe] or [CHd] because the appropriate model provided better agreement with certain precise experimental data; though no guarantee exists whether it will work equally well for other sets of experiments.) For polycrystals, however, the basic element is naturally predetermined from the very internal structure—this is just the single grain (see Section 1.6). The latter perhaps explains why the SCS provides as a rule more accurate predictions for the effective properties of polycrystals than of particulate media.

Note finally that the self-consistent method can be employed in an obvious manner to multiphase media as well. However, its predictions will possess the needed symmetry (2.65) only when the dispersed inclusions are aligned and of similar shape, see the paper [BEe] for details, examples and comments on this important fact.

1.5.3.2 An Alternative Derivation

Eq. (5.20) can be also recast as

$$\frac{\overline{\kappa(\boldsymbol{x}) - \kappa^*}}{\kappa(\boldsymbol{x}) + 2\kappa^*} = 0, \quad (5.21)$$

where the overbar indicates, let us recall, averaging over the RVE, and $\kappa(\boldsymbol{x})$ is the function that takes the values κ_1 or κ_2 depending on whether \boldsymbol{x} lies in the constituent ‘1’ or ‘2’, respectively. Eq. (5.21) has a simple and clear interpretation. Namely, imagine that the RVE, \mathcal{V} , is filled with spherical particles, whose sizes vary from finite down to infinitesimal. The spheres have conductivity κ_1 or κ_2 . Imagine each

sphere lying in a homogeneous medium with the effective conductivities κ^* ; at infinity the prescribed temperature gradient \mathbf{G} is imposed. The deviation from this gradient within the sphere, due to the fact that its properties differ from those of the surrounding material, is just

$$\frac{\kappa(\mathbf{x}) - \kappa^*}{\kappa(\mathbf{x}) + 2\kappa^*} \mathbf{G}, \quad (5.22)$$

cf. Eqs. (1.14) and (1.15). (In the electrostatic context, the latter value is proportional to the so-called polarization of the sphere.) Since the volume \mathcal{V} is considered as macroscopically homogeneous, we should have, accordingly, *no* macroscopical polarization. The mean value of the “local” polarizations (5.22) should then vanish, as claimed in Eqs. (5.20) and (5.21).

The above reasoning can be interpreted as well in the following manner, that represents a modification of the original Maxwell arguments of Section 1.1.3.3. Cut again a big sphere of the radius A (the “Maxwell sphere”) from the heterogeneous medium and immerse it into unbounded homogeneous host material whose conductivity κ^+ will be appropriately chosen (or, so to say after Berryman [BEM], “tuned”). “Sit down” at the point M far away, i.e. at the distance R from the center of the sphere, $R \gg A$. Let the temperature field $\mathbf{G} \cdot \mathbf{x}$ be applied at infinity. Each piece of the phases ‘1’ or ‘2’, located in the vicinity of \mathbf{x} , will create at the point M the disturbance

$$\frac{a^3}{R^3} \frac{\kappa(\mathbf{x}) - \kappa^+}{\kappa(\mathbf{x}) + 2\kappa^+} \mathbf{G}, \quad (5.23)$$

—since we are far from the piece under consideration, it can be taken as spherical with a radius a . Averaging (5.23) over the big heterogeneous sphere will give a quantity, proportional to

$$\frac{\kappa(\mathbf{x}) - \kappa^+}{\kappa(\mathbf{x}) + 2\kappa^+}. \quad (5.24)$$

Comparing (5.24) with (5.21) shows that if we “tune” the host medium so that $\kappa^+ = \kappa^*$, the presence of the heterogeneous sphere will not be “felt” at the point M ; in other words this sphere will become “transparent” for us.

The above arguments represent a “static” (and scalar) implementation of Berryman’s idea [BEM]: this author dealt with the long-wave length limit for a harmonic wave, scattered by the “Maxwell

sphere,” and “tuned” the properties of the host medium in such a way that the total scattering is zero—in other words, the sphere becomes indeed invisible for us. Similar arguments in the language of the so-called T -matrix were employed in [GUa], [KOa].

Remark 5.9 Sometimes the SC scheme is called the *Coherent Potential Approximation* due to the similarity of its implementation (cf. Eq. (5.24)) to a certain approach, used in the theory of electronic properties of imperfect crystals and alloys, see [PAb] or the excellent exposition in Ziman’s book [ZIa].

1.5.3.3 The Percolation Phenomenon

Going back to the simplest SCS equation (5.19), note that it possesses the simple solutions

$$\frac{\kappa^*}{\kappa_1} = \begin{cases} \frac{1}{1 - 3\phi_2}, & \text{if } \kappa_2/\kappa_1 = \infty, \\ 1 - \frac{3}{2}\phi_2, & \text{if } \kappa_2/\kappa_1 = 0, \end{cases} \quad (5.25)$$

in the two limiting cases of ideally conducting particles ($\kappa_2/\kappa_1 = \infty$) or non-conducting particles ($\kappa_2/\kappa_1 = 0$), respectively.

Hence, a dispersion of ideally conducting spheres becomes ideally conducting, if the volume fraction $\phi_2 \geq 1/3$, whatever the conductivity of the matrix, the spatial distribution of the spheres and their sizes. This is just an exhibition of the so-called *percolation phenomenon* and the value ϕ_2^p ($1/3$ for the adopted SCS) is the *percolation threshold*. The essence of the phenomenon is the following: when an ideally conducting constituent ‘2’ is added to a poorly conducting matrix, it is most possible that it will be in the form of separated particles, if the volume concentration ϕ_2 is small enough. When increasing ϕ_2 , the particles start touching each other, forming more complicated aggregates. At certain critical (threshold) value ϕ_2^p , the constituent ‘2’ forms a continuous skeleton penetrating the whole body of the mixture and as a result it becomes ideally conducting as well. A similar percolation phenomenon appears obviously in the case when a nonconducting phase ($\kappa_2 = 0$) is added to a conducting matrix. In this case the threshold concentration $\phi_2^p = 2/3$, again *independently* of microstructural details, see Eq. (5.25).

It is noted that the percolation phenomena are very important in solid state physics, in general, and in many of its applications. The appropriate discussion goes however far beyond the scope of the present work (see the survey [LAc] or [KIa] for basic ideas, results and classical references).

Remark 5.10 *In the literature the presence of a percolation threshold is sometimes considered as a virtue of an approximate model, while its lack (in the differential scheme below, for example) is viewed as a drawback (or vice versa, depending on author's taste). It should be noted that the threshold's presence (or lack) has nothing in common with the validity of the model. It only informs us that for the geometry that realizes the model (like Milton' SCS-geometry), there is (or there is not) a threshold. Hence this is a conclusion concerning above all a specific two-phase geometry, but not a model or its applicability.*

1.5.3.4 Some Particular Cases

Consider now, for illustration, several particular cases of the SCS equations (5.18).

- For *randomly oriented and isotropic spheroids*, in the scalar conductivity case,

$$\frac{\kappa^*}{\kappa_1} = 1 + \frac{[\kappa]}{3\kappa_1} \left(\frac{2\kappa^*}{\kappa^* + (\kappa_2 - \kappa^*)M_\perp} + \frac{\kappa^*}{\kappa^* + (\kappa_2 - \kappa^*)M} \right) \phi_2, \quad (5.26)$$

cf. Eqs. (4.21) and (5.18). When the spheroids are spheres, $M = M_\perp = \frac{1}{3}$, and (5.26) reproduces (5.19).

- Let $\kappa_2 = 0$, and the spheroids degenerate into *penny-shaped cracks*. The effective conductivity κ^* is then eliminated from the right-hand side of Eq. (5.26) and Eq. (5.12) is recovered, but without the correction term $\mathcal{O}(\varepsilon)$, cf. Eq. (5.9). Hence the self-consistent scheme predicts the linear dependence

$$\frac{\kappa^*}{\kappa_1} = 1 - \frac{8}{9}\varepsilon \quad (5.27)$$

of κ^* upon the crack density parameter.

The results in the *elastic case* are obtained in a fully similar way, and we shall only list some of the basic ones.

- For an isotropic *elastic dispersion of spheres*, the self-consistent scheme yields

$$\begin{aligned} k^* &= k_1 + k^* \frac{k_2 - k_1}{k^* + \alpha^*(k_2 - k^*)} \phi_2, \\ \mu^* &= \mu_1 + \mu^* \frac{\mu_2 - \mu_1}{\mu^* + \beta^*(\mu_2 - \mu^*)} \phi_2, \\ \alpha^* &= \frac{3k^*}{3k^* + 4\mu^*}, \quad \beta^* = \frac{6}{5} \frac{k^* + 2\mu^*}{3k^* + 2\mu^*}, \end{aligned} \quad (5.28)$$

see Eqs. (5.18) and (4.58). This is an algebraic system with respect to the unknown effective moduli k^* and μ^* which allows a convenient numerical solution (by a straightforward iterative procedure).

The system (5.28) is usually attributed to Budiansky [BUa] and Hill [HIe], see also [WUa]. (These authors were apparently not aware of the earlier Skorohod's paper [SKa], where the same classical self-consistent reasoning was employed to derive (5.28).)

Very simple closed form solutions (5.28) can be found, if $\nu_1 = \nu_2 = 0.2$. Then, as pointed out by Budiansky [BUa], the Poisson ratio of the medium is also 0.2, $\alpha^* = \beta^* \equiv 0.5$.

Other simple solutions exist if the Poisson ratio of the matrix is again $\nu_1 = 0.2$, but the inclusions are rigid or represent voids. In particular, for spherical voids in a matrix of Poisson ratio $\nu_1 = 0.2$, the solution of (5.28) is extremely simple

$$\begin{aligned} \frac{\kappa^*}{\kappa_1} &= \frac{\mu^*}{\mu_1} = 1 - 2\phi_2 \quad (k_2 = \mu_2 = \infty), \\ \frac{\kappa^*}{\kappa_1} &= \frac{\mu^*}{\mu_1} = \frac{1}{1 - 2\phi_2} \quad (k_2 = \mu_2 = 0), \end{aligned} \quad (5.29)$$

and hence $\nu^* \equiv 0.2$ in both cases.

The foregoing facts suggest that the value 0.2 of the Poisson ratio is something special in the “one-particle” models of particulate media.¹⁴ A certain explanation can be sought perhaps in the fact that

¹⁴It was Hashin [HAc] who first pointed out the “curious” fact that $\nu^* \equiv 0.2$ in a dilute dispersion of rigid spheres in a matrix for which $\nu_1 = 0.2$.

at $\nu_1 = 0.2$ the concentration factor for a single spherical inclusion—the tensor \mathbb{A}_w , as given in Eq. (4.58), is proportional to the unit fourth-rank tensor \mathbb{I} .

Eq. (5.29) means that for a dispersion of spheres, in a matrix with $\nu_1 = 0.2$, the percolation threshold, as predicted by SCS, is $\phi_2^p = 0.5$. At sphere fractions, higher than 0.5, the solid either become rigid or cannot sustain load. Again, this fact is neither a merit or a fault of the SCS, but just a property of the special Milton’s SCS-geometry that “lies” behind the scheme.

Another simple solution of (5.28) emerges for the Hill medium, when the shear moduli of the phases coincide, $\mu_1 = \mu_2 = \mu$. Then, from the first equation, one has

$$\frac{k^* - k_1}{k_2 - k_1} = \phi_2 \frac{3k^* + 4\mu}{3k_2 + 4\mu}. \quad (5.30)$$

which reproduces the Hill formula (3.66). Hence the SCS gives the exact value of the effective bulk modulus in the case of spherical particles. (Recall, however, that the Hill results (5.30) holds for an arbitrary two-phase geometry, which is macroscopically isotropic.)

- For an isotropic elastic solid, containing *randomly oriented penny-shaped cracks*, we get formally the same system (5.17), with the only difference that the Poisson ratio of the matrix, ν_1 , is replaced by this ratio of the composite medium, ν^* :

$$\begin{aligned} \frac{k^*}{k_1} &= 1 - \frac{16}{9} \frac{1 - \nu^{*2}}{1 - 2\nu^*} \varepsilon, \\ \frac{\mu^*}{\mu_1} &= 1 - \frac{32}{45} \frac{(1 - \nu^*)(5 - \nu^*)}{2 - \nu^*} \varepsilon. \end{aligned} \quad (5.31)$$

This is exactly the self-consistent system of Budiansky and O’Connell [Bub] for the effective moduli of a microcracked solid (cf. their Eqs. (36) and (44')).

1.5.4 The Differential Scheme

The differential scheme (DS) is a kind of an “infinitesimal” implementation of the self-consistent idea. It was initiated by Bruggeman [BRf], [BRg] and used in fifties for media containing rigid particles (by Brinkman [BRb] for the viscosity of a fluid suspension, and by

Roscoe [ROa] in the elastic case). More recently it was elaborated by McLaughlin [MCb], Norris [NOa], Zimmerman [ZIC] *et al.* A detailed discussion can be found in the survey [CLb].

1.5.4.1 The Basic Idea

Imagine the small concentration $\delta\Gamma$ of particles is added to an initially homogeneous medium. Replace mentally the so obtained mixture by a homogeneous medium of the effective conductivity $\mathbf{K}^* = \mathbf{K}^*(\delta\Gamma)$. In the latter a new concentration $\delta\Gamma$ of particles is inserted; the new medium again is replaced by a homogeneous one of conductivity $\mathbf{K}^*(2\delta\Gamma)$, and so forth. As a result, the effective conductivity will be a certain function of the total amount Γ of inserted particles, $\mathbf{K}^* = \mathbf{K}^*(\Gamma)$. Since at each step a small concentration of particles is added, $\delta\Gamma \ll 1$, the dilute approximation (5.1) applies

$$\mathbf{K}^*(\Gamma + \delta\Gamma) = \mathbf{K}^*(\Gamma) + \delta\Gamma (\kappa_2 \mathbf{I} - \mathbf{K}^*(\Gamma)) \cdot \mathbf{A}_w(\mathbf{K}^*(\Gamma), \kappa_2).$$

In the limit $\delta\Gamma \rightarrow 0$, this yields the differential equation

$$\frac{d\mathbf{K}^*}{d\Gamma} = (\kappa_2 \mathbf{I} - \mathbf{K}^*(\Gamma)) \cdot \mathbf{A}_w(\mathbf{K}^*(\Gamma), \kappa_2) \quad (5.32)$$

for the unknown function $\mathbf{K}^* = \mathbf{K}^*(\Gamma)$, which should be solved together with the natural initial condition

$$\mathbf{K}^*(0) = \kappa_1 \mathbf{I}.$$

The reasoning in the elastic case is fully similar, and will be omitted.

It is very important to point out, after McLaughlin [MCb], that the total concentration Γ of particles, introduced into the matrix, *does not coincide* with the volume concentration ϕ_2 of the second phase. The reason is that when adding a new portion $\delta\Gamma$ of particles, some of them will “fall” within the region, occupied by the previously deposited ones. Only the part $\phi_1 \delta\Gamma$, that “falls” within the matrix, will increase ϕ_2 . Thus, in the limit $\delta\Gamma \rightarrow 0$ again,

$$d\phi_2 = (1 - \phi_2) d\Gamma \quad \text{or} \quad \Gamma = -\ln(1 - \phi_2), \quad (5.33)$$

because, obviously, $\Gamma = 0$ at $\phi_2 = 0$. From (5.33) it follows that

$$\Gamma = \phi_2 + \frac{1}{2}\phi_2^2 - \dots,$$

which means that $\Gamma \approx \phi_2$ for $\phi_2 \ll 1$. Hence only for small values of ϕ_2 one can choose $\Gamma = \phi_2$.

Remark 5.11 *In some of the earlier papers [HEa], [ZIb], the differential scheme was applied without distinguishing between the quantity Γ and the fraction ϕ_2 . One of the motivation was Mackenzie's treatment of a porous solid [MAa], in which a new single pore is added at the center of a sphere, cut from the homogenized medium, and subjected to hydrostatic pressure. As just pointed out, taking $\Gamma = \phi_2$ is safe only in the dilute case; for higher values of ϕ_2 the deviations from the differential scheme's predictions is already considerable.*

Obviously, the phases do not enter symmetrically in the Eqs. (5.32) and (5.33), unlike the self-consistent scheme. On the other hand again the effective medium surrounding of the inclusion is imagined at each step of the DS procedure. That is why the DS is often called, after Landauer [LAc], the *Second Bruggeman's unsymmetrical Effective Medium Approximation*. Also the term *iterated dilute limit approximation* is sometimes used, which reflects well the reasoning that has led us to the formulae (5.32) and (5.33).

The differential scheme, similarly to the self-consistent one, is a realizable approximation in the sense that there exist special two-phase media whose effective behavior coincides exactly with the predictions of the scheme. This important fact was first demonstrated by Norris *et al.* [NOa], [NOb], [NOc], see also [AVa].

1.5.4.2 Some Particular Cases

Consider now in more detail the system (5.32) and (5.33) in several particular cases.

- For *spherical inclusions in the scalar conductivity context* the tensor $\mathbf{K}^* = \kappa^* \mathbf{I}$ is isotropic and \mathbf{A}_w is given in (4.13). Eq. (5.32) then becomes

$$\frac{df}{d\phi_2} = \frac{3(\alpha - f(\phi_2))f(\phi_2)}{(1 - \phi_2)(\alpha + 2f(\phi_2))}, \quad \kappa^*/\kappa_1 = f(\phi_2), \quad (5.34)$$

$\alpha = \kappa_2/\kappa_1$. Similarly to the self-consistent scheme, Eq. (5.34) allows simple solutions

$$\frac{\kappa^*}{\kappa_1} = \begin{cases} \frac{1}{(1 - \phi_2)^3}, & \text{if } \kappa_2/\kappa_1 = \infty, \\ (1 - \phi_2)^{3/2}, & \text{if } \kappa_2/\kappa_1 = 0, \end{cases} \quad (5.35)$$

in the two limiting cases of ideally conducting particles ($\kappa_2/\kappa_1 = \infty$) or non-conducting particles ($\kappa_2/\kappa_1 = 0$), respectively. Hence, there is no percolation in the differential scheme—the values of κ^* remain finite and positive for all $\phi_2 \in (0, 1)$.

- For *spherical inclusions in the elastic case* the DS supplies the system

$$\begin{aligned} \frac{1}{k^*} \frac{dk^*}{d\phi_2} &= \frac{(3k^* + 4\mu^*)(k_2 - k^*)}{(1 - \phi_2)k^*(3k_2 + 4\mu^*)}, \\ \frac{1}{\mu^*} \frac{d\mu^*}{d\phi_2} &= \frac{5(3k^* + 4\mu^*)(\mu_2 - \mu^*)}{(1 - \phi_2)(6\mu^*(k^* + 2\mu^*) + (9k^* + 8\mu^*)\mu^*)}, \end{aligned} \quad (5.36)$$

coupled with the obvious initial conditions $k(0) = k_1$, $\mu(0) = \mu_1$. The system (5.36) was derived by McLaughlin [MCb] who showed, in particular, that its solution meets the HS bounds.¹⁵

A detailed analysis of the system (5.36) was performed by Zimmerman [Zic]. He observed that (5.36) is autonomous, with the parameter Γ , see Eq. (5.33), playing the role of time. This suggests to divide the equations of (5.36) and the result will be an explicit, though complicated, expression of ϕ_2 through the ratio k^*/μ^* (or which is the same, through the effective Poisson ratio ν^*). Simpler solutions exist in the limiting cases of rigid and vacuous inclusions. The equation for ν^* that follows from (5.36) has in these cases the form

$$\frac{d\nu^*}{d\Gamma} = F(\nu_1)(1 - 5\nu_1).$$

Though the function $F(\nu_1)$ is different for rigid and vacuous inclusions, the presence of the multiplier $1 - 5\nu_1$ in both cases assures that $\nu^* \equiv 0.2$, if $\nu_1 = 0.2$ —something that is identical with the predictions of the SCS. Moreover, the value 0.2 of the Poisson ratio is an *attractor* or a *fixed point*, in the sense that the function $\nu^* = \nu^*(\phi_2)$ is monotonically increasing, if $\nu^*(0) = \nu_1 < 0.2$, and monotonically decreasing, if $\nu^*(0) = \nu_1 > 0.2$. In both cases $\nu^*(\phi_2) \rightarrow 0.2$ as $\phi_2 \rightarrow 1$. The same attractor's type behavior has been observed in the SCS by the author [MAd].

¹⁵Once an approximate scheme is realizable, its predictions always satisfy the HS bounds, due to the optimality of the latter; see Section 1.3.3.

Remark 5.12 *It is curious to understand whether the peculiarity of the value 0.2 for the Poisson ratio is something that indeed exists in real heterogeneous solids, or it is a mathematical artifact produced by the models. This intriguing question explains the considerable interests in the last 15 years in studying the so-called Poisson ratio flow diagrams i.e. the effective Poisson coefficient as a function of the volume fraction ϕ_2 of the inclusions. It turned out that if the inclusions are voids, the fixed points on such diagrams (like the above value 0.2) do exist, and this was demonstrated both analytically (see, e.g. [CHb] in 2-D) and numerically by a number of authors. Details, discussion and many references can be found in the recent paper [CHf].*

For rigid inclusions it seems as if there are no fixed points for the Poisson ratio, as numerical experiments suggest, see again [CHf]. The apparent discrepancy between voids and rigid inclusions may be however a by-product of the numerical procedures, employed by the authors. After Zimmerman [ZId], one can point out that calculations for a medium with “vacuous pores” can be performed simply putting the elastic moduli $\kappa_2 = \mu_2 = 0$ in the appropriate equations and numerical schemes. But the analogous calculations for rigid inclusions are performed taking the moduli κ_2, μ_2 very large, but still finite. One should be very careful, dealing with limit of moduli, tending both to zero and to infinity. The problem arises because, when taking either limit 0 or ∞ , any references of the Poisson ratio may be lost. In fact, one can construct paths $\kappa_2, \mu_2 \rightarrow 0$ or ∞ in (κ_2, μ_2) -space so that the Poisson ratio can have any value. For more details, concerning this subtle situation, the reader is referred to the original paper [Zid].

Another similarity with the SCS is the existence of the simple solutions of (5.36), when $\nu_1 = 0.2$, for the two limiting types of inclusions, namely

$$\begin{aligned} \frac{k^*}{k_1} = \frac{\mu^*}{\mu_1} &= (1 - \phi_2)^2 \quad (\text{voids}), \\ \frac{k^*}{k_1} = \frac{\mu^*}{\mu_1} &= \frac{1}{(1 - \phi_2)^2} \quad (\text{rigid inclusions}), \end{aligned} \tag{5.37}$$

cf. Eq. (5.35).

Remark 5.13 *Relations of the type $(1 - \phi_2)^m$ for the decrease of a certain effective property of a porous solid as a function of the*

void ratio ϕ_2 are very popular and useful in some applications like micromechanics of microporous rocks. (In this context m is known as the cementation exponent and its value supplies additional microstructural information, see [SEa] for details and references.) They are often called Archie's after the work [ARa]. The reappearance of the phenomenological Archie's law within the DS, cf. (5.35) and (5.37), cannot be interpreted, however, as a kind of justification of the scheme or as an indication of its superiority as compared to other approximate theories. It means solely that the specific two-phase Norris' microgeometry that "lies" behind the DS, exhibits Archie's type behavior of its effective conductivity and elasticity (for $\nu_1 = 0.2$ in the latter case).

Another particular case, in which the system (5.36) possesses a very simple solution, is when both the matrix and spheres are rigid. Then $k_1 = k_2 = k^* = \infty$ and

$$\frac{\mu^*}{\mu_1} = \frac{1}{(1 - \phi_2)^{5/2}} \quad (5.38)$$

which reproduces the Einstein formula (1.21) in the dilute limit (recalling once again the full mathematical analogy between an incompressible elastic solid and a fluid in Stokesian approximation). The formula (5.38) was proposed by Brinkman [BRb] for the viscosity of a fluid suspension, within his attempt of extending the Einstein formula (1.21) in nondilute case. To this end the author has utilized literally the same DS reasoning of Section 1.5.4.1.

We shall skip further study of the DS model and equations, referring to the already cited papers of McLaughlin, Norris *et al.* and Zimmerman. Also the application of the DS to the microcracked solids will not be discussed (in this case some care is needed, due to the "degenerated" nature of the inclusions). Details and further references can be found in the Hashin paper [HAj], see also [HEa].

1.5.5 The Effective Field

Here again each particle is treated as single. However, we imagine it immersed now into a homogeneous medium possessing the properties of the matrix. The influence of the rest of the particles is accounted for through the assumption that the particle lies within

a certain external field—the effective field—that *differs* from the applied macroscopic one. Similarly to the self-consistent scheme, this is an old approach that goes back to the Mossotti cavity idea and to the Lorenz-Lorentz local field, as we shall point out below.

1.5.5.1 The Basic Idea

We shall first implement the effective field idea again in the scalar case. Let \mathbf{G}^* be the local (effective, or Lorenz-Lorentz' in the dielectric context) field that acts on each particle; in this simplest version it is assumed that \mathbf{G}^* is a constant.

Since each particle is lying as single in the field, it is natural also to assume that

$$\langle \nabla \theta \rangle_1 = \mathbf{G}^* . \quad (5.39)$$

As a matter of fact, this is the *basic assumption* of the simplest version of the effective field method—it states that each particle undergoes an external field that *coincides* with the mean field in the matrix phase.

In turn, \mathbf{G}^* should depend linearly on the applied macroscopic gradient $\mathbf{G} = \overline{\nabla \theta}$

$$\mathbf{G}^* = \mathbf{B} \cdot \mathbf{G} , \quad (5.40)$$

with a certain second-rank tensor \mathbf{B} . The latter is specified by means of (5.39) and the first equation of (2.35):

$$\begin{aligned} \mathbf{G} = \overline{\nabla \theta} &= \phi_1 \langle \nabla \theta \rangle_1 + \phi_2 \langle \nabla \theta \rangle_2 \\ &= \phi_1 \mathbf{G}^* + \phi_2 \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot \mathbf{G}^* \\ &= (\phi_1 \mathbf{I} + \phi_2 \mathbf{A}_w(\kappa_1, \mathbf{K}_2)) \cdot \mathbf{G}^* ; \end{aligned} \quad (5.41)$$

we have used that $\langle \nabla \theta \rangle_2 = \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot \mathbf{G}^*$ since each particle is treated as single in the far-field \mathbf{G}^* , according to the basic assumption. Hence

$$\mathbf{B} = (\phi_1 \mathbf{I} + \phi_2 \mathbf{A}_w(\kappa_1, \mathbf{K}_2))^{-1} , \quad (5.42)$$

which gives explicitly the tensor \mathbf{B} that interconnects the applied macroscopic field and the resulting local one.

The concentration tensor can be easily found now by means of (5.41) and (5.42):

$$\begin{aligned} \langle \nabla \theta \rangle_2 &= \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot \mathbf{G}^* \\ &= \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot \mathbf{B} \cdot \mathbf{G} = \mathbf{A}_2 \cdot \mathbf{G} , \end{aligned}$$

so that, in virtue of (5.42),

$$\mathbf{K}^* = \kappa_1 \mathbf{I} + \phi_2 \mathbf{A}_w(\kappa_1, \mathbf{K}_2) \cdot (\phi_1 \mathbf{I} + \phi_2 \mathbf{A}_w(\kappa_1, \mathbf{K}_2))^{-1} \quad (5.43)$$

which is the *effective field approximation* for the bulk conductivity of the medium.

In the elastic case, fully similar arguments produce the formula

$$\mathbb{L}^* = \mathbb{L}_1 + \phi_2 \mathbb{A}_w(\mathbb{L}_1, \mathbb{L}_2) : (\phi_1 \mathbb{I} + \phi_2 \mathbb{A}_w(\mathbb{L}_1, \mathbb{L}_2))^{-1}, \quad (5.44)$$

having replaced the second-rank tensors in (5.43) by the appropriate fourth-rank tensors.

1.5.5.2 Alternative Derivations and Interpretations

Note first that the formula (5.41) and its consequences (5.43) and (5.44) for the effective properties has an appealing interpretation in terms of the Mossotti cavity idea (see Section 1.1.3.2). Indeed, guided by the heuristic derivation of the Clausius-Mossotti formula, as used by Feynman *et al.* [FEc, Chapter 11], let us cut the inclusions, treated as isolated, from the medium and replace them by cavities. Then

$$\mathbf{G} = \mathbf{G}_{\text{cav}} + \mathbf{G}_{\text{incl}}, \quad (5.45)$$

where \mathbf{G}_{cav} is the field in the matrix with cavities and, correspondingly, \mathbf{G}_{incl} is the field that appears in the inclusions. The “cavity” field \mathbf{G}_{cav} is $\mathbf{G}_{\text{cav}} = \phi_1 \mathbf{G}^*$, where \mathbf{G}^* is the above mentioned mean (or effective) field that results from the interactions of the inclusions. In turn, $\mathbf{G}_{\text{incl}} = \phi_2 \mathbf{A}_w \cdot \mathbf{G}^*$, since each one is treated as isolated in the far-field \mathbf{G}^* . Together with (5.45), these formulae reproduce the basic relation (5.41) of the effective field method.

An approach which turns out to be closely connected, if not equivalent, to the effective field approximation is associated with the names of Mori and Tanaka [MOB] in the literature on composites, see also [BEc], [WEa], [WEb] *et al.* The original derivation of these authors was expressed in terms of eigenstrains, equivalent inclusions, transformation energy consideration, etc., and at first glance looked totally different in spirit from the rest of the models, used in mechanics of heterogeneous media. (Details and further applications can be found in the book of Mura [MUa].) The clarification of the nature of this approximation is to be attributed to Benveniste who, in the paper

[BEd], pointed out that the basic idea of Mori-Tanaka’s method is just the statement of Eq. (5.39), namely, that each particle is again treated as single, but lying within the far-field $\langle \nabla \theta \rangle_1$ that equals the mean field in the matrix. This assumption was adopted also by the author in the note [MAe], without any connection to Mori-Tanaka’s work, as a starting point of the derivation of the approximations (5.43) and (5.44) for the effective moduli, as given in Section 1.5.5.1.

As we shall see below, the effective field method works well and produces reasonable results in the cases when the inclusions are either spherical or, if nonspherical, are aligned. For multi-phase systems with different alignment and/or shape of the particles, the effective field predictions fail to satisfy the necessary symmetry conditions (2.65) and thus they are not acceptable, see [BEe], [FEb]. The same shortcoming of the SCS was already pointed out in Remark 5.8.

This failure, in particular, suggests that the effective field method should be modified for media with more complicated internal structure. A possible way was proposed by Kanaun and Levin in a number of publications and elaborated in their book [KAf], see also [KAg] for a detailed English exposition. Using the integral equation for the displacement field in a particulate medium, they have derived an approximate “self-consistent” equation for the effective field. The solution of the latter, though simple, involves however “two-point correlation” functions for the inclusions’ distribution. For spherical particles, isotropically distributed, the Kanaun-Levin’s scheme yields the same results (5.46) and (5.47), given below as particular cases of the foregoing effective field (Mori-Tanaka) method. Details and some of the latest results, concerning the application of this approach to scalar waves phenomena in particulate media, can be found in Chapter 3 of this volume.

1.5.5.3 Some Particular Cases

Consider again some of the most common and interesting particular cases, to illustrate the predictions of the effective field method.

- Let the medium be a macroscopically isotropic *random dispersion of spheres*. The tensors \mathbf{A}_w and \mathbb{A}_w are given in Eqs. (4.13) and (4.58) respectively, so that the effective field prescriptions (5.43) and (5.44) yield

$$\frac{\kappa^*}{\kappa_1} = 1 + \frac{3\beta\phi_2}{1 - \phi_2\beta}, \quad \beta = \frac{[\kappa]}{\kappa_2 + 2\kappa_1}, \quad (5.46)$$

in the scalar case, and

$$\frac{k^*}{k_1} = 1 + \frac{\phi_2[k]}{k_1 + \alpha_1 \phi_1[k]}, \quad \frac{\mu^*}{\mu_1} = 1 + \frac{\phi_2[\mu]}{\mu_1 + \beta_1 \phi_1[\mu]}, \quad (5.47)$$

in the elastic case; the parameter α_1 and β_1 are defined in Eq. (4.58).

The formula (5.46) reproduces the Maxwell one, cf. Eq. (1.19), which in turn coincides with the appropriate Hashin-Shtrikman bound (3.34).

Similarly to the scalar case, the formulae (5.47) provide bounds on the elastic moduli of a two-phase material in the “well-ordered” case (see Section 1.3.5). Indeed, the expression for the bulk modulus in (5.47) obviously coincides with one of the Hashin-Shtrikman bounds on k^* , as given in (3.68). Similarly, the expression for μ^* in the same formula (5.47) is the HS-bound [HAM], which is upper, if $k_2 > k_1$, $\mu_2 > \mu_1$ and lower, if both inequality signs are reversed.

It is noted that the formulae (5.47) were also derived by Kuster and Toksöz in the paper [KUc] (which is most often cited in geophysical community, but almost unknown outside it). The method employed there is a direct generalization of the “Maxwell sphere,” treated in the scalar context in Section 1.1.3.3. Here the long-wavelength scattering by a “big” sphere, containing a host of small inhomogeneities, was evaluated in two different ways: (i) taking the spheres as homogeneous with unknown effective moduli and, (ii) summing the scattering waves from all small particles. Equating these quantities reproduces (for spherical shape of the latter) the formula (5.47), see also Berryman’s discussion in [BEm], [BEn].

- For a *fiber reinforced material*—circular cylinders, aligned along the axis Ox_3 , the tensors \mathbf{A}_w and \mathbb{A}_w , as given in Eqs. (4.15) and (4.62), respectively, are utilized.

In the scalar case the effective conductivity tensor is transversely isotropic and has the form (5.5). The transverse conductivity reads

$$\frac{\kappa_{11}^*}{\kappa_1} = 1 + \frac{2\beta\phi_2}{1 - \phi_2\beta}, \quad \beta = \frac{[\kappa]}{\kappa_2 + \kappa_1}, \quad (5.48)$$

which is the 2-D counterpart of the Maxwell formula (1.19). Note that the latter also provides a bound on κ^* for an arbitrary macroscopically isotropic 2-D mixture.

For the conductivity along the fibers we have the same formula as in (5.6), i.e. the Voigt value $\kappa_{33}^* = \bar{\kappa} = \kappa^v$ (and this is fully natural, because the temperature gradient along the fibers is homogeneous).

In the elastic case the fiber-reinforced material under study is again transversely isotropic and thus it is characterized macroscopically by means of five elastic moduli. Utilizing Hill's notations (4.60) and (4.61), with Eq. (4.62) for the tensor \mathbb{A}_w inserted into the formula (5.44) for \mathbb{L}^* , we get, after some algebra:

$$\begin{aligned} \mathbb{L}^* &= (2k^*, \ell^*, \ell^*, n^*, 2m^*, 2\mu^*), \\ k^* &= \lambda_1 + \mu_1 + \frac{\phi_2 \gamma_1}{\Delta} ([\lambda] + [\mu]), \quad \ell^* = \lambda_1 + \mu_1 \frac{\phi_2 \gamma_1 [\lambda]}{\Delta}, \\ n^* &= \gamma_1 + \phi_2 [\gamma] - \phi_1 \phi_2 \frac{[\lambda]^2}{\Delta}, \\ m^* &= \mu_1 \left(1 + \frac{\phi_2 [\mu]}{\mu_1 + \phi_1 \chi_1 [\mu]} \right), \\ \mu^* &= \mu_1 \left(1 + \frac{2\phi_2 [\mu]}{2\mu_1 + \phi_1 [\mu]} \right), \end{aligned} \tag{5.49}$$

with the notations

$$\begin{aligned} \Delta &= \phi_1(\lambda_2 + \mu_2) + \phi_2(\lambda_1 + \mu_1) + \mu_1, \\ \chi_1 &= \frac{\lambda_1 + 3\mu_1}{2(\lambda_1 + 2\mu_1)} = \frac{3 - 4\nu_1}{4(1 - \nu_1)}. \end{aligned} \tag{5.50}$$

The above expressions (5.49) for the moduli k^* , ℓ^* , n^* , m^* and μ^* coincide with those found by Hashin and Rosen [HAn], see also [Hic]. In their derivation, Hashin and Rosen used the exact 2-D counterpart of the Hashin assemblage (see Section 1.3.4)—i.e. a medium, consisting of parallel “composite cylindrical elements” (a cylindrical core of one of the constituents, coated with a concentric shell of the other, in such a way that the volume fractions ϕ_1 and ϕ_2 are fixed). They also showed that the value of μ^* , as given in Eq. (5.49), lies within the rigorous bounds, derived in the same paper [HAn]. The formulae (5.49) were rederived by Levin [LEb] as well, who employed, in a quite complicated way, a version of the effective field method, see also [KAf].

• In a similar manner one can treat a medium, containing *identical, but randomly oriented spheroidal inhomogeneities*. The scalar conductivity of such a medium, according to Eqs. (4.23) and (5.43), reads

$$\kappa^* = \kappa_1 + \frac{\phi_2[\kappa]\gamma_\Omega}{\phi_1 + \phi_2\gamma_\Omega}, \quad (5.51)$$

where γ_Ω depends on the shape of the spheroid through its depolarization factors M and M_\perp , as seen from the formula (4.23).

Remark 5.14 *The formula (5.51) in an equivalent form, was proposed by Fricke [FRa]. In this work, and in a series of papers that followed, the author compared some accurate experimental results with the prediction of (5.51), using data for conductivity of dog's blood. The red corpuscles were approximated as identical, but randomly oriented spheroids, and Fricke found that the best fit to experiments corresponds to the choice of prolate spheroidal form, when (in our notations) $c/a = 4.25$. These papers of Fricke are in a sense certain natural extension of Einstein's idea, already discussed in Section 1.1.3.4: while the latter looked only for the size of the particles in a solute by means of micromechanical experiment, the former was interested in more specific details, like the particle shape (assuming it spheroidal which, of course, is by no means obvious). A number of new methods of such "micromechanical" nature, that are able to provide information about the microstructure of a dispersion (connected, e.g. with sedimentation, diffusion, etc.), were developed later on. Some ideas, results and references can be found in [JEb], where polydisperse materials were treated by means of the notion of the so-called effective diameter.*

The elastic moduli of the same dispersion of spheroids are

$$k^* = k_1 + \frac{\phi_2[k]a'}{\phi_1 + \phi_2a'}, \quad \mu^* = \mu_1 + \frac{\phi_2[\mu]a''}{\phi_1 + \phi_2a''}, \quad (5.52)$$

see (5.44) and (4.66), with the parameters a' and a'' , defined in (4.67).

• Consider finally the most interesting particular case of a *micro-cracked solid*, when the spheroids degenerate into randomly oriented penny-shaped cracks (with their conductivity and elastic moduli vanishing at the same time).

In the scalar case Eq. (5.51) yields in this limiting case

$$\frac{\kappa^*}{\kappa_1} = \frac{1}{1 + \delta}, \quad \delta = \lim_{\xi \rightarrow 0} \phi_2 \gamma_\Omega,$$

where $\xi = c/a$, see the end of Section 1.4. The quantity δ in the last formula was evaluated in Eq. (5.10) and the result, let us recall, is $\delta = \frac{8}{9}\varepsilon$. Hence

$$\frac{\kappa^*}{\kappa_1} = \frac{1}{1 + \frac{8}{9}\varepsilon}, \quad (5.53)$$

where ε is the crack density parameter, cf. (5.11).

Remark 5.15 *As shown recently by the author [MAf], the approximation (5.53) provides an upper bound on the effective conductivity of the solid, if (i) there is no correlation between the location and the orientation of the cracks and, (ii) The distance between the centers of the cracks is greater than $2a$ (which means that overcrossing of is forbidden, whatever the orientations, with cracks' centers fixed). We recall that a denotes the radius of the penny-shaped cracks under consideration.*

For an elastic microcracked solid the formula (5.52) yields

$$\frac{k^*}{k_1} = 1 - \frac{\phi_2 a'}{1 + \phi_2 a'}, \quad \frac{\mu^*}{\mu_1} = 1 - \frac{\phi_2 a''}{1 + \phi_2 a''},$$

in which the limit $\xi = c/a \rightarrow 0$ should be taken once again. But the appropriate limits were already evaluated in the dilute case, cf. Eq. (5.17). Hence, the effective field predictions for the elastic moduli of a microcracked solid read

$$\begin{aligned} \frac{k^*}{k_1} &= \frac{1}{1 + \frac{16}{9} \frac{1 - \nu_1^2}{1 - 2\nu_1} \varepsilon}, \\ \frac{\mu^*}{\mu_1} &= \frac{1}{1 + \frac{32}{45} \frac{(1 - \nu_1)(5 - \nu_1)}{2 - \nu_1} \varepsilon}. \end{aligned} \quad (5.54)$$

The formulae (5.54) were proposed by Benveniste [BEd] within the frame of Mori-Tanaka's approximation (see also [BEc] for the 2-D

case—a microcracked plane). A thorough discussion of this approximation with many appropriate references, can be found in Kachanov’s survey [KAa]. Note that the foregoing coincidence of the Benveniste results with Eq. (5.54) is fully natural, having in mind the already pointed out equivalence of the Mori-Tanaka’s scheme and the effective field idea, in its simplest form treated here. It turned out also that the values (5.54), similarly to the scalar case, cf. Remark 5.15, provide upper bounds on the effective elastic moduli of the microcracked solid, under the conditions (i) and (ii) of the same remark, see [MAf].

1.5.6 The Conductivity of a Medium with Nonideal Interphase Contacts

In the case of thermally nonideal interphase contacts, the “one-particle” approximations can be constructed in a manner, fully similar to the ideal contacts’ case, treated in the foregoing analysis. The only difference is that the formulae (2.50) and (2.53) should be employed instead of (2.41), thus taking into account the “surface concentration factors” $\mathbf{A}^{(12)}$ and $\mathbf{B}^{(12)}$, as defined in Eqs. (2.49) and (2.52).

The simplest case of spherical inclusions will be treated again for illustration, within the frame of the self-consistent approach. The formulae (4.38) and (4.44), valid for a single sphere, allow us to obtain then the surface concentration factors

$$\mathbf{A}^{(12)} = \phi_2 \mathbf{A}_s^{(12)}(\kappa^*, \kappa_2), \quad \mathbf{B}^{(12)} = \phi_2 \mathbf{B}_s^{(12)}(\kappa^*, \kappa_2),$$

having imagined that each sphere lies in a matrix with unknown conductivity κ^* , cf. (2.49) and (2.52). Recalling (4.13) and inserting the explicit expressions for $\mathbf{A}_s^{(12)}$ and $\mathbf{B}_s^{(12)}$ from the same formulae in (2.50) and (2.53), respectively, gives the *self-consistent equations*

$$\kappa^* = \kappa_1 + 3\phi_2 \kappa^* \left(\frac{[\kappa]}{\kappa_2 + 2\kappa^*} + \frac{2C\kappa^*}{\kappa_2 + 2(1+C)\kappa^*} \right) \quad (5.55)$$

in the superconducting case, and

$$\kappa^* = \kappa_1 + 3\phi_2 \kappa^* \left(\frac{[\kappa]}{\kappa_2 + 2\kappa^*} - \frac{2R\kappa_1}{\kappa_2 + 2(1+R)\kappa^*} \right) \quad (5.56)$$

in the resistance case.

With the same ease the rest of the above discussed approximate schemes of “one-particle” type can be implemented. Some other examples of similar schemes with more detailed exposition, discussion, comparison with experiments, etc., can be found, e.g. in the papers [HAo], [HAp], [BEb], [MIa] *et al.* Variational principles and estimates, accounting for nonideal contacts, are given, for instance, in the papers [TOd], [LIa], which also include a number of appropriate and useful references.

Here it suffices perhaps to demonstrate briefly only two specific effects in two-phase media that stem out from the nonideal interphase contacts.

First, imagine that the inclusions are highly conducting, $\alpha = \kappa_2/\kappa_1 \rightarrow \infty$, but the thermal resistance of the contacts is very high at the same time, $R \rightarrow \infty$, with the ratio $\chi = R/\alpha$ remaining finite. The formula (5.56) then gives

$$\frac{\kappa^*}{\kappa_1} = \frac{1}{1 - 3\phi_2(1 - \chi)}.$$

This relation, for small to moderate values of ϕ_2 , is in a reasonable agreement with experimental data of De Araujo and Rosenberg [DEa] and the appropriate lower bound of Torquato and Rintoul [TOd].

Second, assume that particles of higher conductivity are distributed in a matrix, i.e. $\alpha > 1$. Then

$$\kappa^* = \kappa_1, \quad \text{if } R = R_c = \frac{1}{6}(\alpha - 1)(\alpha + 2), \quad (5.57)$$

as it follows again from (5.56). The above means that at $R = R_c$ the thermal resistance of the interphases “hides” the inclusions, so that macroscopically their presence is not felt at all. This fact is directly connected with the presence of the so-called “critical radius” a_c , see [CHc], [EVa] *et al.* The essence is that the interfacial effects are *size-dependent*: the radius a enters the definitions of both interfacial characteristics C and R , cf. their definitions (4.26) and (4.28) (or (4.27)) respectively. In particular, whatever be the fixed volume fraction ϕ_2 , Eq. (4.28) implies that when decreasing the particles’ radius a , we shall reach a value $a = a_c$ —the *critical radius*—for which R coincides with the value R_c , given in (5.57). Then the “bad” interphase will produce enough resistance to compensate for the higher conductivity of the inclusions. The effective conductivity, as a result, will not be able to exceed that of the matrix, when $a \leq a_c$.

Torquato and Rintoul [TOd] have shown that the value of $R_c = \alpha - 1$ *exactly* for a dispersion of nonoverlapping spheres. The foregoing self-consistent scheme gave a totally different value of R_c (see Eq. (5.57)). This fact demonstrates once again that the self-consistent reasoning, though based on consideration of a single inclusion in a homogeneous medium, has, in reality, little in common with dispersions of equi-sized particles.

Note finally that in the papers [KAd], [KAe] the thermoelastic properties of composites (dispersion of spheres) with nonideal contacts were studied in detail by means of the effective field method.

1.5.7 The Self-consistent Scheme for the Absorption Problem

To illustrate the generality of the “one-particle” approximations, we shall discuss here a self-consistent type scheme for evaluating the effective sink strength. Recall that this problem, motivated in particular by the classical Smoluchowski’s work [SMa], was discussed in Section 1.2.7. It is specified by Eqs. (2.66) and (2.67). The scheme to be applied is due to Brailsford and Bullough [BRa]. The implementation follows Talbot and Willis [TAb].

The self-consistent scheme provides an approximation for $\langle c \rangle_2$ assuming that each inclusion is single and it is immersed into a medium of the effective sink strength k^{*2} . Hence, choosing for simplicity the inclusions’ shape spherical (of the radius a), one should solve the “single inclusion problem” which, in the present context reads:

$$\begin{aligned} \Delta c(\mathbf{x}) - k_2^2 c(\mathbf{x}) + K &= 0, & \text{if } r < a, \\ \Delta c(\mathbf{x}) - k^{*2} c(\mathbf{x}) + K &= 0, & \text{if } r > a. \end{aligned} \tag{5.58}$$

Due to the radial symmetry of the problem, the solution has the form

$$c(\mathbf{x}) = \begin{cases} \frac{K}{k_2^2} + \frac{A \sinh k_2 r}{k_2 r}, & r < a, \\ \frac{K}{k^{*2}} + \frac{B e^{-k^* r}}{k^* r}, & r > a. \end{cases}$$

The constants A and B are fixed by the conditions that both the function $c(\mathbf{x})$ and its normal derivative dc/dr on the sphere $r = a$

should be continuous. The calculations, though tedious, are straightforward, and the final result for $c(\boldsymbol{x})$, together with (2.73), yields eventually

$$\begin{aligned} & \frac{k^{*2} - k_1^2}{k_2^2 - k_1^2} \tag{5.59} \\ &= \frac{\phi_2}{k_2^2} \left\{ k^{*2} + 3 \frac{(k_2^2 - k^{*2})(1 + k^*a)(k_2a \cosh k_2a - \sinh k_2a)}{(k_2a)^2(k^*a \sinh k_2a + k_2a \cosh k_2a)} \right\}. \end{aligned}$$

This cubic (with respect to the dimensionless quantity k^*a) equation is the absorption counterpart of the self-consistent equations (5.19) and (5.28) for the conductivity and the elastic moduli, respectively. Similarly to them, Eq. (5.59) does not pretend to be exact, since spheres' interactions are not taken into account with due precision, but only approximately. Nevertheless, it allows to reveal certain interesting features of the absorption problem's homogenization, that distinguish the latter from that of the more "ordinary" scalar and elastic problems.

Consider first the limiting case, when

$$k_1a \rightarrow 0, \quad k_2a \rightarrow 0. \tag{5.60}$$

The solution of Eq. (5.59) is then $k^{*2} = k_v^{*2} = \phi_1 k_1^2 + \phi_2 k_2^2$. This is just the Voigt type approximation, already observed in the scalar and elastic cases, and also in the absorption problem under study, see Eq. (3.78). Recall that it corresponds to the assumption that the concentration field $c(\boldsymbol{x})$ remains constant in \mathcal{V} . It is noted, after Talbot and Willis [TA], that the formula (3.78) is fully natural in the case under study. Indeed, the limits (5.60) mean that, at fixed k_1 and k_2 , the radius of the inclusions decreases to zero. The fluctuation of the field $k^2(\boldsymbol{x})$, as defined in (2.68), becomes then more and more rapid, $c(\boldsymbol{x})$ has, so to say, little chance to vary and remains approximately constant. A rigorous justification of the foregoing reasoning, i.e. the validity of the Voigt's type formula (3.78) in the case (5.60) is due to Papanicolaou [PAa].

In the other limiting case, when

$$k_1a \rightarrow \infty, \quad k_2a \rightarrow \infty, \tag{5.61}$$

Eq. (5.59) generates now the Reuss type formula $k^{*2} = k_r^2$, see Eq. (3.79). The physical explanation of this result is also transparent

enough [TAb]. The limit (5.61) means that at fixed k_1^2 and k_2^2 the spheres' radius increases. The matrix-inclusion interrelations affect then only thin boundary layers, elsewhere $c \equiv K/k_1^2$ or $c \equiv K/k_2^2$ within the phase 1' and 12' respectively. Thus

$$\bar{c} = \frac{K}{k^{*2}} = \frac{\phi_1 K}{k_1^2} + \frac{\phi_2 K}{k_2^2},$$

which does yield (3.79).

The foregoing results indicate that the elementary bounds (3.80) are sharp, in the sense that they cannot be improved.

Hence in both limiting cases Eq. (5.59) is exact. The most interesting range is therefore $k_1 a$, $k_1 a \sim \mathcal{O}(1)$, since the interactions then become of crucial importance, and the exact spatial distribution of the sinks cannot be neglected. We shall illustrate this fact, again qualitatively, on the classical Smoluchowski's problem (see Section 1.1.3) that corresponds to the "hard" limit (2.69) of Eq. (2.66). In this case the self-consistent equation (5.59) becomes

$$(1 - \phi_1)(k^* a)^2 = 3\phi_1(1 + k^* a)$$

whose elementary solution, when expanded as a series for small values of ϕ_2 , reads

$$k^{*2} a^2 = 3\phi_2 + 3\sqrt{3}\phi_2^{3/2} + \dots,$$

or

$$\frac{k^{*2}}{k_s^2} = 1 + \sqrt{3\phi_2} + \frac{5}{2}\phi_2 + \dots, \quad (5.62)$$

where k_s^2 is the Smoluchowski's value of the effective absorption, valid in the dilute limit, see Eq. (1.24) (at $D = 1$).

The formula (5.62) demonstrates an interesting and important feature of the Smoluchowski problem, namely, that the effective absorption coefficient k^{*2} represents a *nonanalytic* function of the concentration ϕ_2 of the trapping inclusions. (The expansion (5.62) suggests, but does not prove of course, that instead it maybe an analytical function of $\sqrt{\phi_2}$.) This fact sharply contrasts the scalar and elasticity counterparts, as well as the absorption problem Eq. (2.66) for any other case, different from the "hard" limit.

The explanation of the nonanalytic dependence (5.62) lies in the appearance of the so-called "screening" (or shielding) effect which

becomes of predominant importance in the Smoluchowski problem. Roughly speaking, this means that a trap will absorb the particles close to it, so that fewer of them can reach other traps “behind” to be “eaten” by them. Such a screening effect is very important also in systems of charged particles (the *Debye shielding*), see e.g. [VAa, Chapter 8.1].

The first several terms of the expansion (5.62) have been obtained, bounded by means of variational procedures and discussed by a number of authors [FEa], [TAa], [TOc], see also [CAa] and Torquato’s survey in the present volume. An interesting approach to the problem is the so-called “point-particle” approximation in which the traps are replaced by appropriate point-sources whose intensity is looked for from a natural consistency condition [FEa]. The same approach is also useful for particulate media in studying their effective elastic properties; see [KAf, Chapter 5.14].

A final remark in this Section is warranted. Everywhere in the foregoing considerations we have considered 3-D heterogeneous media. The 2-D case can be treated as well—a natural interpretation will be provided by a medium containing an array of infinite cylindrical inclusions, parallel to a fixed axis, when the applied temperature gradient or external loading is perpendicular to it. In the conductivity and elastic contexts, all 2-D counterparts of the 3-D considerations and results can be repeated straightforwardly which explains their omission here.

There exists however a notable exception when the 2-D situation is drastically different from its 3-D analog. It concerns the Smoluchowski problem in 2-D, when the inclusions represents a sparse system of aligned circular cylinders. In this case the solution of the Laplace equation (1.23) in 2-D contains the function $\ln r/a$, instead of a/r , and hence the condition $c(r) \rightarrow c_0$ as $r \rightarrow \infty$ *cannot* be satisfied. (Note that the situation here is fully similar to the well-known Stokes paradox [HAa, Chapter 2.7], which “assures” us that there exists no Stokesian flow, bounded at infinity, around a cylinder.)

The nonexistence of the single-cylinder solution in the case under study does not mean of course that the effective absorption coefficient k^*2 cannot be defined. It only implies that the interactions are so strong here, that a dilute formula, like the Smoluchowski one (1.25),

cannot be found.¹⁶ The dependence k^{*2} upon ϕ_2 will be proportional, say, to $\ln \phi_2$ even for $\phi_2 \ll 1$. (Such logarithmic dependencies do appear in homogenization problems with very strong interactions—an example is provided by the very interesting and important problem, concerned with the effective permeability of a randomly perforated membrane, which however cannot be discussed here even briefly, see, e.g. [MAc] and the references therein.

1.6 Elastic Properties of Polycrystals

We shall present here some basic ideas and simplest results concerning the application of one of the approximate schemes of the previous Section for predicting the effective properties of polycrystals. This is the oldest scheme in the field—the self-consistent—proposed by Hershey [HEb] and Kröner [KRd]. As an illustration only the cubic symmetry case will be treated in more detail.

1.6.1 The Self-Consistent Scheme for Polycrystals

The polycrystal is an assembly of monocrystals—homogeneous grains with one and the same elastic properties, defined by the elastic tensor \mathbb{L} . The crystallographic axes of each grain vary. Hence the tensor \mathbb{L} is “rotated” in a complicated manner when one moves across the solid and exactly this is what makes the polycrystal heterogeneous. For simplicity sake and to avoid cumbersome details that may eclipse the clarity of the basic ideas, we assume that there exist no preferable orientations of grains, i.e. of the crystallographic axes. Hence there is no texture presented so that the polycrystal is macroscopically isotropic, with a tensor of effective moduli

$$\mathbb{L}^* = 3k^* \mathbb{I}' + 2\mu^* \mathbb{I}'' ,$$

where \mathbb{I}' and \mathbb{I}'' are the two basic fourth-rank isotropic tensors, defined in Eq. (4.58). Our aim is to develop a certain simple approximate

¹⁶This explains the failure in 2-D of certain variational procedures for estimating k^{*2} for random dispersions; see the recent author’s lecture [MAG] for details and references.

scheme of self-consistent type for evaluating \mathbb{L}^* by means of the given elastic tensor \mathbb{L} for a single grain.

Imagine each grain is a sphere, immersed into an unbounded matrix with the effective, but yet unknown, properties \mathbb{L}^* . Fix one of the grains, \mathcal{W} . According to Eqs. (4.10) and (4.55) the strain within such a grain is constant

$$\boldsymbol{\varepsilon}_{\text{gr}} = \mathbb{A}_w(\mathbb{L}, \mathbb{L}^*) : \boldsymbol{E}, \quad (6.1)$$

where $\boldsymbol{E} = \bar{\boldsymbol{\varepsilon}}$ is the prescribed macrostrain tensor, applied to the polycrystalline RVE. Moreover, in virtue of Eqs. (4.7), (4.55) and (4.58)

$$\begin{aligned} \mathbb{A}(\mathbb{L}, \mathbb{L}^*) &= \mathbb{A}^* = [\mathbb{I} + \mathbb{P}^* : (\mathbb{L} - \mathbb{L}^*)]^{-1}, \\ \mathbb{P}^* &= p_1^* \mathbb{I}' + p_2^* \mathbb{I}'' , \\ p_1^* &= \frac{1}{3k^* + 4\mu^*}, \quad p_2^* = \frac{3}{5\mu^*} \frac{k^* + 2\mu^*}{3k^* + 4\mu^*}. \end{aligned} \quad (6.2)$$

(The subscript ‘ w ’ will be suppressed from now on.) The asterisk everywhere underlines that the appropriate quantities, like p_1^* , etc., are evaluated by means of the effective elastic moduli k^* , μ^* of the polycrystal.

Note that in writing Eqs. (6.1) and (6.2) we have used the fact the the formula (4.55) is applicable under the *sole* assumption that the matrix is isotropic; the anisotropy of the inclusion can be at the same time arbitrary, as pointed out in Section 1.4.

Let us now average Eq. (6.1) with respect to all possible crystallographic orientations of the axes of the grain. (This operation will be denoted by $\langle \cdot \rangle_{\Omega}$, similarly to Section 1.4). Then

$$\langle \boldsymbol{\varepsilon}_{\text{gr}} \rangle_{\Omega} = \langle \mathbb{A}^* \rangle_{\Omega} : \bar{\boldsymbol{\varepsilon}}, \quad (6.3)$$

The *key* observation now is the identity

$$\langle \boldsymbol{\varepsilon}_{\text{gr}} \rangle_{\Omega} = \bar{\boldsymbol{\varepsilon}} \quad (6.4)$$

i.e. the average (with respect to all crystallographic orientations) strain in a grain *equals* the macrostrain.

Remark 6.1 *Assuming all grains spherical we have a kind of Hashin’s assemblage (Section 1.3.3)—a set of spheres of different sizes, from*

finite down to infinitesimal, filling the RVE, \mathcal{V} . The spheres differ (mechanically) only in crystallographic orientation so that, averaging over the latter, we should get the macrostrain. (Observe that the strain-concentration factor \mathbb{A} in Eq. (6.1) does not depend on the grain size.)

Inserting (6.3) into (6.4), one gets the basic self-consistent equation

$$\langle \mathbb{A}^* \rangle_{\Omega} = \mathbb{I}, \quad (6.5)$$

through which the unknown effective tensor \mathbb{L}^* can be found; \mathbb{I} is the unit fourth-rank tensor that appeared in Eq. (4.55).

An equivalent to Eq. (6.5) formulation follows, if one applies the tensor \mathbb{L} to both parts of Eq. (6.1), evaluating thus the stress tensor within a grain:

$$\boldsymbol{\sigma}_{\text{gr}} = \mathbb{L} : \boldsymbol{\varepsilon}_{\text{gr}} = \mathbb{L} : \mathbb{A}^* : \bar{\boldsymbol{\varepsilon}},$$

and average the result with respect to all possible orientations:

$$\langle \boldsymbol{\sigma} \rangle_{\Omega} = \langle \mathbb{L} : \boldsymbol{\varepsilon}_{\text{gr}} \rangle_{\Omega} = \langle \mathbb{L} : \mathbb{A}^* \rangle_{\Omega} : \bar{\boldsymbol{\varepsilon}}. \quad (6.6)$$

But, similarly to Eq. (6.4), observe that

$$\langle \boldsymbol{\sigma}_{\text{gr}} \rangle_{\Omega} = \bar{\boldsymbol{\sigma}} = \mathbb{L}^* : \bar{\boldsymbol{\varepsilon}}$$

which, together with Eq. (6.6), yields the equation

$$\mathbb{L}^* = \langle \mathbb{L} : \mathbb{A}^* \rangle_{\Omega}, \quad (6.7)$$

equivalent to the self-consistent one (6.5).

Remark 6.2 *The equivalence of Eqs. (6.5) and (6.7) can be formally demonstrated in a simple way, using the expression for the tensor \mathbb{A}^* , see (6.2). Indeed, from this expression we have*

$$[\mathbb{I} + \mathbb{P}^* : (\mathbb{L} - \mathbb{L}^*)] : \mathbb{A}^* = \mathbb{I}$$

which, when averaged over orientations, yields

$$\langle \mathbb{A}^* \rangle_{\Omega} + \mathbb{P}^* : \langle \mathbb{L} : \mathbb{A}^* \rangle_{\Omega} - \mathbb{P}^* : \mathbb{L}^* : \langle \mathbb{A}^* \rangle_{\Omega} = \mathbb{I},$$

or

$$\mathbb{I} - \langle \mathbb{A}^* \rangle_{\Omega} = \mathbb{P}^* : \left[\langle \mathbb{L} : \mathbb{A}^* \rangle_{\Omega} - \mathbb{L}^* : \langle \mathbb{A}^* \rangle_{\Omega} \right]. \quad (6.8)$$

Now, if Eq. (6.5) holds, i.e. $\langle \mathbb{A}^* \rangle_\Omega = \mathbb{I}$, then Eq. (6.8) immediately implies (6.7). Conversely, if Eq. (6.7) holds, then $\langle \mathbb{L} : \mathbb{A}^* \rangle_\Omega = \mathbb{L}^*$ and (6.8) becomes

$$\mathbb{I} - \langle \mathbb{A}^* \rangle_\Omega = \mathbb{P}^* : \mathbb{L}^* : \left[\mathbb{I} - \langle \mathbb{A}^* \rangle_\Omega \right],$$

i.e. $\mathbb{I} - \langle \mathbb{A}^* \rangle_\Omega = 0$ which is exactly the needed Eq. (6.5).

Other equivalent forms of the self-consistent equation (6.5) have been proposed by Kröner [KRe]. He then ingeniously exploited them to bound the effective properties for a polycrystal, using simple algebraic arguments.

1.6.2 Formulation in Compliances and Consistency of the Scheme

Let

$$\boldsymbol{\sigma}_{\text{gr}} = \mathbb{B}^* : \bar{\boldsymbol{\sigma}}, \quad \mathbb{B}^* = \mathbb{B}_w(\mathbb{M}, \mathbb{M}^*), \quad (6.9)$$

be the solution of the single sphere (i.e. single grain) problem in stresses; $\mathbb{M} = \mathbb{L}^{-1}$ and \mathbb{M}^* are the compliance tensors of the grain and of the polycrystal respectively. Recall that both stress and strain tensors $\boldsymbol{\varepsilon}_{\text{gr}}$ and $\boldsymbol{\sigma}_{\text{gr}}$ are constant within the (spherical) grain under study. Upon comparing Eqs. (6.1) and (6.9) we find that

$$\mathbb{A}^* = \mathbb{M} : \mathbb{B}^* : \mathbb{M}^{*-1} \quad \text{or} \quad \mathbb{M} : \mathbb{B}^* = \mathbb{A}^* \mathbb{M}^*. \quad (6.10)$$

We employ again the reasoning of Section 1.6.1, but with respect to stresses now. That is, average Eq. (6.9) with respect to all grain's orientations:

$$\langle \boldsymbol{\sigma}_{\text{gr}} \rangle = \langle \mathbb{B}^* : (\mathbb{M}, \mathbb{M}^*) \rangle : \bar{\boldsymbol{\sigma}}$$

and note that $\langle \boldsymbol{\sigma}_{\text{gr}} \rangle = \bar{\boldsymbol{\sigma}}$. Then the self-consistent equation for the effective compliance tensor \mathbb{M}^* emerges

$$\langle \mathbb{M}^* \rangle_\Omega = \mathbb{I}, \quad (6.11)$$

which is the natural counterpart of Eq. (6.5). An equivalent formulation reads

$$\mathbb{M}^* = \langle \mathbb{M} : \mathbb{B}^* \rangle_\Omega. \quad (6.12)$$

The latter can be obtained, say, if one applies the tensor \mathbb{M} to both parts of Eq. (6.9) to get the strain $\boldsymbol{\varepsilon}_{\text{gr}} = \mathbb{M} : \boldsymbol{\sigma}_{\text{gr}}$ in the grain, and then average this result with respect to all crystallographic orientations.

Theorem 6.1 Eqs. (6.5) and (6.11) are equivalent, in the sense that

$$\mathbb{L}^* : \mathbb{M}^* = \mathbb{I}, \quad (6.13)$$

i.e. the effective properties of the polycrystal, calculated by means of the above described self-consistent procedure, are the same, no matter whether the schemes, based on elastic moduli or compliances, are utilized.

Proof. Let \mathbb{M}^* be the effective compliance, as calculated from (6.11). Denote $\mathbb{L}^+ = \mathbb{M}^{-1}$ and average Eq. (6.10) over all orientations:

$$\langle \mathbb{A}(\mathbb{L}, \mathbb{L}^+) \rangle_{\Omega} : \mathbb{M}^* = \langle \mathbb{M} : \mathbb{B}^* \rangle_{\Omega} = \mathbb{M}^*,$$

having used Eq. (6.12). Thus $\langle \mathbb{A}(\mathbb{L}, \mathbb{L}^+) \rangle_{\Omega} = \mathbb{I}$; comparing the latter with Eq. (6.5) that specifies \mathbb{L}^* , one concludes that indeed $\mathbb{L}^+ = \mathbb{L}^* = \mathbb{M}^{*-1}$. \square

1.6.3 Example: Elastic Moduli of a Cubic Polycrystal

The tensor of the elastic moduli \mathbb{L} in this simplest case is

$$\mathbb{L} = 3k\mathbb{I}' + 2\mu_2\mathbb{I}'' + 2(\mu_1 - \mu_2)\mathbb{O}_h, \quad (6.14)$$

where

$$\mathbb{O}_h = \mathbf{e}_1^4 + \mathbf{e}_2^4 + \mathbf{e}_3^4 \quad (6.15)$$

is the basic fourth-rank tensor with cubic symmetry (whose axes are along the orthonormal crystallographic basis \mathbf{e}_i , $i = 1, 2, 3$, see [SPa]). For this simplest anisotropy, the effective bulk modulus coincides with that of the grains:

$$k^* = k + \frac{2}{3}(\mu_1 - \mu_2), \quad (6.16)$$

because if the applied stress tensor is spherical. the strain is a pure dilatation, one and the same in all grains. To simplify the calculation of the shear modulus, introduce three basic fourth-rank tensor with cubic symmetry as follows

$$\boldsymbol{\Sigma}_1 = \mathbb{I}', \quad \boldsymbol{\Sigma}_2 = \mathbb{I}' + \mathbb{I}'' - \mathbb{O}_h, \quad \boldsymbol{\Sigma}_3 = \mathbb{O}_h - \mathbb{I}'. \quad (6.17)$$

It is easily checked that they are orthogonal, in the sense that

$$\begin{aligned} \boldsymbol{\Sigma}_i : \boldsymbol{\Sigma}_j &= 0, \quad i \neq j, \\ \boldsymbol{\Sigma}_i : \boldsymbol{\Sigma}_j &= \boldsymbol{\Sigma}_i, \quad i = 1, 2, 3 \quad (\text{no sum over } i). \end{aligned} \quad (6.18)$$

In the sequel, the symbolic notation

$$\mathbb{L} = (\alpha, \beta, \gamma) \Leftrightarrow \mathbb{L} = \alpha \boldsymbol{\Sigma}_1 + \beta \boldsymbol{\Sigma}_2 + \gamma \boldsymbol{\Sigma}_3 \quad (6.19)$$

will be useful. The isotropic tensors are characterized by the equality $\beta = \gamma$, i.e. they have the form (α, β, β) . The most important formula, however, concerns the tensors of the form (6.19), averaged over orientation; it reads, symbolically,

$$\langle \mathbb{L} \rangle_{\Omega} = \langle (\alpha, \beta, \gamma) \rangle_{\Omega} = (\alpha, \bar{\beta}, \bar{\beta}), \quad \bar{\beta} = \frac{1}{5}(3\beta + 2\gamma). \quad (6.20)$$

It is a straightforward consequence of the fact that $\langle \mathbb{O}_h \rangle_{\Omega} = \frac{1}{5} \mathbb{H}$, where \mathbb{H} is the fully-symmetric isotropic fourth-rank tensor, defined in (4.56); the multiplier $1/5$ follows from a full contraction of both sides of (6.20), having noticed that $\langle \mathbb{O}_h \rangle_{\Omega}$ is proportional to \mathbb{H} . Hence

$$\langle \mathbb{O}_h \rangle_{\Omega} = \frac{1}{5} [2\mathbb{I} + 3\mathbb{I}'] = \mathbb{I}' + \frac{2}{5}\mathbb{I}''.$$

According to the definitions (6.17) of the basic tensors $\boldsymbol{\Sigma}_2$ and $\boldsymbol{\Sigma}_3$, we have

$$\langle \boldsymbol{\Sigma}_2 \rangle_{\Omega} = \frac{3}{5}\mathbb{I}'', \quad \langle \boldsymbol{\Sigma}_3 \rangle_{\Omega} = \frac{2}{5}\mathbb{I}'',$$

and (6.20) immediately follows from the last two equations.

For the tensor \mathbb{L} of a single grain, see (6.14), we have

$$\mathbb{L} = (\alpha, \beta, \gamma), \quad \alpha = 3k^*, \quad \beta = 2\mu_2, \quad \gamma = 2\mu_1. \quad (6.21)$$

Due to the ‘‘orthogonal’’ properties (6.18) of the basic tensors $\boldsymbol{\Sigma}_i$, $i = 1, 2, 3$, the multiplication and inversion of the tensors in the symbolic form (6.19) is extremely simple. Namely,

$$\mathbb{L} = (\alpha, \beta, \gamma) \Rightarrow \mathbb{L}^{-1} = (1/\alpha, 1/\beta, 1/\gamma),$$

$$\mathbb{L}' = (\alpha', \beta', \gamma'), \quad \mathbb{L}'' = (\alpha'', \beta'', \gamma'') \Rightarrow \mathbb{L}' : \mathbb{L}'' = (\alpha' \alpha'', \beta' \beta'', \gamma' \gamma'').$$

Due to Eqs. (6.2) and (6.21) we thus have

$$\begin{aligned} & \mathbb{I} + \mathbb{P}^* : (\mathbb{L} - \mathbb{L}^*) \\ &= (1, 1, 1) + (p_1^*, p_2^*, p_2^*) \cdot \left[(3k^*, 2\mu_2, 2\mu_1) - (3k^*, 2\mu^*, 2\mu^*) \right] \\ &= (1, 1 + 2p_2^*(\mu_2 - \mu^*), 1 + 2p_2^*(\mu_1 - \mu^*)), \end{aligned}$$

so that,

$$\begin{aligned} \langle \mathbb{A} \rangle_{\Omega} &= \left\langle \left[\mathbb{I} + \mathbb{P}^* : (\mathbb{L} - \mathbb{L}^*) \right]^{-1} \right\rangle_{\Omega}, \\ \delta &= \frac{3}{5} \frac{1}{1 + 2p_2^*(\mu_2 - \mu^*)} + \frac{2}{5} \frac{1}{1 + 2p_2^*(\mu_1 - \mu^*)}. \end{aligned} \quad (6.22)$$

Here

$$2p_2^* = \frac{3}{5\mu^*} \frac{k^* + 2\mu^*}{3k^* + 4\mu^*} \quad (6.23)$$

in virtue of Eq. (6.2) and k^* is the bulk modulus of the polycrystal, given in (6.16). It remains to recall the self-consistent condition (6.5) $\langle \mathbb{A}^* \rangle_{\Omega} = \mathbb{I} = (1, 1, 1)$ which means that the unknown shear modulus μ^* solves the equation $\delta = 1$, with δ defined in (6.22). Using (6.23) we recast this equation, after some algebra, to its final form:

$$\begin{aligned} \left(\frac{\mu^*}{\mu_1} \right)^3 + a \left(\frac{\mu^*}{\mu_1} \right)^2 - b \left(\frac{\mu^*}{\mu_1} \right) - c &= 0, \\ a = \frac{9k^* + 4\mu_1}{8\mu_1}, \quad b = \frac{3\mu_2(k^* + 4\mu_1)}{8\mu_1^2}, \quad c = \frac{3k^*\mu_2}{4\mu_1^2}. \end{aligned} \quad (6.24)$$

It is easy to see that if $k, \mu_1, \mu_2 > 0$, this cubic equation has only one real root, as it should.

Eq. (6.24) was first derived by Hershey [HEb] and, independently, by Kröner [KRd], who developed the self-consistent theory of polycrystals. Details and further references can be found in the reviews [WAb], [KRf], as well as in the book [SHb] (concerned mainly with polycrystals and covering, in particular, the rich Russian literature on the subject).

The experimental data reported and discussed in these references support very favorably the predictions of the self-consistent theory for polycrystals and, in particular, those of Eq. (6.24). This is natural enough, since for polycrystals we have a well-defined basic element to be embedded in an effective medium, namely the single crystallite. For a particulate medium the choice of such an element is not that obvious, and many choices may compete, as already pointed out in Section 1.5.3.1 (see Remark 5.8).

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