CHAPTER 13

Local and Homogenized Equations

Homogenization theory is concerned with finding the appropriate *homogenized* (or averaged, or macroscopic) governing partial differential equations describing physical processes occurring in heterogeneous materials when the length scale of the heterogeneities tends to zero. In such instances it is desired that the effects of the microstructure reside wholly in the *macroscopic* or *effective* properties via certain weighted averages of the microstructure. In its simplest form, the method is based on the consideration of two length scales: the macroscopic scale L, characterizing the extent of the system, and the *microscopic* scale ℓ, associated with the heterogeneities. Moreover, it is supposed that some external field is applied that varies on a *characteristic* length scale Λ. If ℓ is comparable in magnitude to Λ or L, then one must employ a microscopic description, i.e., one cannot homogenize the equations.

The limit of interest for purposes of homogenization is

$$L \geq \Lambda \gg \ell.$$

Therefore, there is a small parameter

$$\epsilon = \frac{\ell}{L}$$

associated with rapid fluctuations in the microstructure or local property. Accordingly, the field quantities (e.g., temperature field, electric field, stress field, concentration field, velocity field) depend on two variables: a *global* or *slow* variable $\boldsymbol{x}$ and a *local* or *fast* variable

$$\boldsymbol{y} = \boldsymbol{x}/\epsilon.$$

The slowly varying parts of the fields are imposed by the source, the boundary conditions, or the initial conditions, while the rapidly varying parts are imposed by the local property or microstructure. These variations are schematically shown in Figure 13.1.
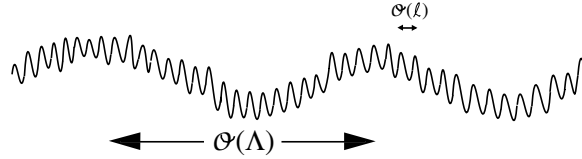
Figure 13.1 A schematic depiction of the slow and rapid parts of the field.

Under these conditions, a complete analysis of the problem involves three steps:

1. One first sets out to find the form of the homogenized or averaged equations, valid on length scales $\mathcal{O}(\Lambda)$, by, for example, performing an asymptotic expansion of the field quantities in terms of the global and local variables. The averaged relations are typically continuum differential equations. This asymptotic analysis is often guided by phenomenology. For example, in the case of electrical (heat) conduction in a heterogeneous material, it is expected that an averaged governing equation applies with an effective conductivity obtainable from an averaged Ohm's (Fourier's) law. Similarly, one seeks an averaged Hooke's law to describe the effective elastic moduli. For flow in porous media, one would like to understand the conditions under which Darcy's law can be derived.

2. Next, one must determine the effective properties that arise in the averaged equations as a function of the microstructure. The quantitative characterization of the microstructure of random media is an enormous subject of research and is dealt with in Part I of this book. The effective properties should mathematically exist as the system volume tends to infinity, independent of the macroscopic boundary conditions.

3. Finally, one must solve the homogenized equations under appropriate boundary or initial conditions.

The remaining chapters in Part II of this book are concerned with methodologies to link the effective properties of a heterogeneous material to its microstructure and the resulting predictions of such structure/property relations.

13.1 Preliminaries

As described in Section 2.1, each realization ω of the two-phase random medium is a domain of space $\mathcal{V} \in \Re^d$. This domain has volume V and is partitioned into two disjoint random sets or phases: phase 1, a domain $\mathcal{V}_1(\omega)$ with volume fraction ϕ_1, and phase 2, a domain $\mathcal{V}_2(\omega)$ with volume fraction ϕ_2. The interface between the two phases is denoted by $\partial \mathcal{V}(\omega)$. Figure 13.2 depicts a schematic of a realization of a two-phase random medium. Ultimately, we are interested in ergodic two-phase random media (Section 2.2.2) and therefore will take the limit $\mathcal{V} \to \Re^d$. Phase i can be a solid, fluid, or void phase characterized by some general constant tensor property $\boldsymbol{K}_i$. Thus, the
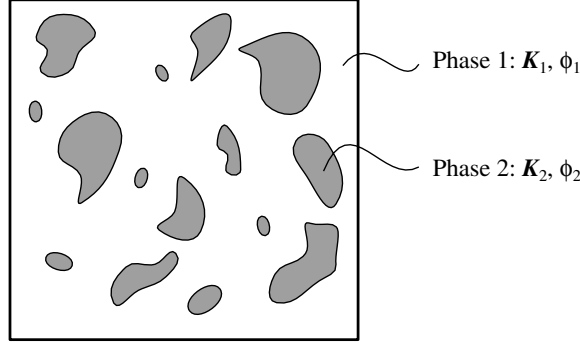
Figure 13.2 A schematic of a realization ω of a two-phase random medium.

associated local property $K(x; \omega)$ at position x in the heterogeneous material can be written in terms of the phase indicator function $\mathcal{I}^{(i)}(x; \omega)$ [cf. (2.1)] as

$$K(x; \omega) = K_1 \mathcal{I}^{(1)}(x; \omega) + K_2 \mathcal{I}^{(2)}(x; \omega). \tag{13.1}$$

This book focuses primarily on four different physical processes: conduction, elasticity, diffusion and reaction among traps, and flow in porous media, together with their associated effective properties. The corresponding *steady-state* effective properties of interest are:

- Effective conductivity tensor, σ_e
- Effective stiffness tensor, C_e
- Mean survival time, τ
- Fluid permeability tensor, k

It will be shown in this chapter that these effective properties of the random heterogeneous material (under certain assumptions about the microstructure) are determined by *ensemble* averages of local fields that satisfy the appropriate conservation equations, i.e., governing partial differential equations.

The claim from Chapter 1 is that any of these effective properties, which we denote generally by K_e, is defined by a linear constitutive relation between an average of a generalized local *flux* F and an average of a generalized local (or applied) *intensity* G, i.e.,

$$F \propto K_e \cdot G. \tag{13.2}$$

Referring to Table 1.1, the effective conductivity tensor σ_e, effective stiffness tensor C_e, mean survival time τ, and fluid permeability tensor k fall within the problem classes A, B, C, and D, respectively. The other problems within the classes are either mathematically analogous or related problems, as will be explained below. Although class A and B problems are of different tensorial order, they share many common features and hence can be attacked using similar techniques. This point is exploited in Chapter 23, where

we obtain cross-property relations involving the effective conductivity on the one hand and effective elastic moduli on the other.

Similarly, despite the fact that the class C trapping problem is a scalar one and the class D flow problem can be either a vector or second-order tensor one, they also share common features, which will be discussed later in this chapter and in Chapter 23 on cross-property relations. It is important to observe that the class A and B problems are considerably different from class C and D problems. Indeed, whereas both the effective conductivity and effective stiffness tensor are scale-invariant properties, both the survival time and fluid permeability are scale-dependent properties. Moreover, unlike class A and B problems, class C and D problems are not characterized by *local properties*; in other words, there is no such thing as a local survival time or a local fluid permeability. This classification scheme is made more mathematically precise in Section 13.6.

In the last two sections we will examine the equations governing certain *time-dependent* trapping and flow problems. In particular, we will define *macroscopic relaxation times* and discuss their relationship to the steady-state mean survival time τ and steady-state fluid permeability $\boldsymbol{k}$.

13.2   Conduction Problem

In this section we begin by stating the local relations for the fields for the conduction problem (Jackson 1990). To motivate the discussion on homogenization, we then describe a model one-dimensional *periodic medium*. The derivation of the homogenized relations in any space dimension d turns out to be somewhat simpler for periodic media than for random media. Accordingly, since the forms of the resulting averaged relations turn out to be identical in both cases, we derive them first in the periodic setting. This is followed by a discussion of the homogenized relations in the random setting.

13.2.1   Local Relations

Consider the steady-state transport or displacement of a conservable quantity associated with any of the class A problems that are summarized in Table 1.1. To fix ideas, we will speak in the language of electrical or thermal conduction, keeping in mind that the results of this section apply as well to the determination of the effective dielectric constant, magnetic permeability, and diffusion coefficient (see Chapter 1 and Section 13.2.5). Each realization ω of the random heterogeneous material that occupies the space $\mathcal{V}$ is composed of two phases (phases 1 and 2) having constant conductivity tensors $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$. In the ensuing discussion, we will temporarily drop ω from the notation.

Local Differential Equations

Let $\boldsymbol{J}(\boldsymbol{x})$ denote the local electric (thermal) current or flux at position $\boldsymbol{x}$, and let $\boldsymbol{E}(\boldsymbol{x})$ denote the local field intensity. Under steady-state conditions with no source terms,

conservation of energy requires that J be solenoidal:

$$\nabla \cdot J(x) = 0 \qquad \text{in } \mathcal{V}, \tag{13.3}$$

for each realization of the ensemble. The intensity field E is taken to be irrotational, i.e.,

$$\nabla \times E(x) = 0 \qquad \text{in } \mathcal{V}, \tag{13.4}$$

which implies the existence of a potential field T, i.e.,

$$E = -\nabla T. \tag{13.5}$$

Thus, E and T represent the electric field (negative of the temperature gradient) and electric potential (temperature) in the electrical (thermal) problem, respectively. We also specify the potential T on the boundary of $\mathcal{V}$. However, we are always ultimately interested in ergodic media and thus in the infinite-volume limit, i.e., $\mathcal{V} \rightarrow \Re^d$. Not surprisingly, we will see that the effective conductivity tensor for this large class of heterogeneous materials exists in this limit and is independent of the boundary conditions on the surface of $\mathcal{V}$ (Papanicolaou and Varadan 1979, Golden and Papanicolaou 1983). This result turns out to be true for all of the other effective properties.

Local Constitutive Relation

In order to close the system of (13.3) and (13.4), we will connect J to E by assuming a linear constitutive relation, i.e.,

$$J(x) = \sigma(x) \cdot E(x) \qquad \text{in } \mathcal{V}, \tag{13.6}$$

where, according to (13.1), the local conductivity tensor can be expressed as

$$\sigma(x) = \sigma_1 \mathcal{I}^{(1)}(x) + \sigma_2 \mathcal{I}^{(2)}(x), \tag{13.7}$$

and $\mathcal{I}^{(i)}(x)$ is the indicator function for phase i given by (2.1). The flux-intensity relation can be expressed in the inverted form

$$E(x) = \rho(x) \cdot J(x) \qquad \text{in } \mathcal{V}, \tag{13.8}$$

where ρ is the second-order *resistivity* tensor. The conductivity and resistivity tensors are related via

$$\rho \cdot \sigma = I, \tag{13.9}$$

where I is the second-order identity tensor, with components, in a rectangular Cartesian coordinate system, given by the *Kronecker delta*

$$\delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & \text{otherwise.} \end{cases} \tag{13.10}$$

It is important to observe that (13.3), which applies anywhere in the heterogeneous material, implies that the normal component of the flux J_n is continuous across the interface $\partial \mathcal{V}$. Similarly, the curl-free condition (13.4) implies that the potential T or,

equivalently, the tangential component of the field E_t is continuous across the interface $\partial \mathcal{V}$. To summarize, the governing equations imply the *ideal* (or *perfect*) interface conditions

$$J_n \text{ and } T \text{ continuous across } \partial \mathcal{V}. \tag{13.11}$$

From a computational viewpoint, the problem can be reformulated as solving (13.3)–(13.6) in *each phase* subject to the interface conditions (13.11) and boundary conditions on the macroscopic sample surface. In general, the tangential component of the flux J_t and the normal component of the field E_n will jump across the interface. Imperfect interfaces (where the potential T jumps across the interface, due to some interfacial resistance, and/or J_n jumps across the interface) were mentioned in Chapter 1.

It is useful to remark on the tensorial nature of the conductivity $\boldsymbol{\sigma}$, which in standard indicial notation is denoted by σ_{ij}. That σ_{ij} is a second-order tensor can be demonstrated by showing that its d^2 components in d dimensions, referred to a coordinate system, transform to d^2 components in another "primed" coordinate system according to the transformation rule for second-order tensors, i.e.,

$$\sigma'_{ij} = l_{ik} l_{jl}\, \sigma_{kl}. \tag{13.12}$$

Here l_{ij} are the direction cosines, i.e., the cosine of the angle between the x_i-axis of the original coordinate system and the x'_j-axis of the new coordinate system. Repeated indices in (13.12) imply summation over all possible values of such indices, i.e.,

$$\sigma'_{ij} = \sum_{k=1}^{d} \sum_{l=1}^{d} l_{ik} l_{jl}\, \sigma_{kl}.$$

If the material admits an *energy density function w* such that the flux (in component form) can be expressed as

$$J_i = \frac{\partial w}{\partial E_i}, \tag{13.13}$$

then it immediately follows from the linear law (13.6) that w, up to an additive constant, is given by

$$w = \frac{1}{2} E_i J_i = \frac{1}{2} E_i \sigma_{ij} E_j \geq 0, \tag{13.14}$$

and thus the conductivity tensor must be symmetric, i.e.,

$$\sigma_{ij} = \sigma_{ji}. \tag{13.15}$$

From relations (13.9) and (13.15), we see that the resistivity tensor $\boldsymbol{\rho}$ must also be symmetric. The symmetry condition (13.15) reduces the number of independent components from d^2 to $d(d+1)/2$. The argument above leading to (13.15) holds for all of the effective properties in class A (Table 1.1). However, in the case of conduction (electrical or thermal) or diffusion processes, the symmetry of the associated effective tensor (transport property) arises directly from Onsager's reciprocity theorem for irreversible

(i.e., dissipative) processes, in which fluxes are linearly related to intensities (Onsager 1931a, Onsager 1931b). This symmetry condition then leads to the energy density function w as given, which physically is the *power dissipation* per unit volume of material. Both the effective dielectric constant and magnetic permeability tensors characterize reversible processes (polarization or magnetization), and therefore the reciprocity theorem does not apply. For such equilibrium properties, w represents the *energy stored* per unit volume of material.

Observe that the nonnegativity of the energy density as expressed by (13.14) places restrictions on the components of $\boldsymbol{\sigma}$ and implies that the conductivity tensor $\boldsymbol{\sigma}$ (or resistivity tensor $\boldsymbol{\rho}$) is *positive definite*. Recall that a symmetric second-order tensor $\boldsymbol{B}$ (B_{ij}) is *positive semidefinite*, if for any vector $\boldsymbol{a}$ (a_i) in $\Re^d$,

$$a_i B_{ij} a_j \geq 0. \tag{13.16}$$

If only the inequality of (13.16) applies for any nonzero vector $\boldsymbol{a} \neq \boldsymbol{0}$, then $\boldsymbol{B}$ is said to be positive definite. Since the equality of (13.14) holds only for $\boldsymbol{E} = \boldsymbol{0}$, $\boldsymbol{\sigma}$ is positive definite, and therefore is also positive semidefinite. (Any positive definite tensor $\boldsymbol{B}$ is also positive semidefinite, since either $\boldsymbol{a} \neq \boldsymbol{0}$ or $\boldsymbol{a} = \boldsymbol{0}$.) Note that for $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$ to be positive definite, it is necessary and sufficient for all of their d real eigenvalues to be positive.

13.2.2   Conduction Symmetry

Conduction symmetry is expressed by the property that the components σ_{ij} (σ_{ij}^{-1}) remain invariant under certain transformations of the coordinates. Basic coordinate changes are (a) reflection in a plane, (b) rotation about an axis, and (c) rotation about an axis combined with reflection in a plane that is normal to the axis. If σ_{ij} (σ_{ij}^{-1}) is invariant to reflection in a plane, then that plane is called a *plane of symmetry*. If σ_{ij} (σ_{ij}^{-1}) is invariant to rotation about an axis, then the axis is one of *rotational symmetry*.

We restrict ourselves initially to three dimensions. In light of the symmetry relation (13.15), the conductivity tensor has only six independent constants:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}. \tag{13.17}$$

We now consider a number of different cases where the tensor σ_{ij} remains invariant to certain transformations according to the rule (13.12). These symmetries result in a reduction in the number of independent components.

(i) Monoclinic Symmetry

For symmetry with respect to one plane, say the x_1-x_2 plane, it can be shown [using relation (13.12)] that σ_{ij} has 4 independent components:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}. \tag{13.18}$$

This is referred to as *monoclinic* symmetry.

(ii) Orthotropic Symmetry

For symmetry with respect to three orthogonal planes, it can be shown [using relation (13.12)] that σ_{ij} has 3 independent components:

$$\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}. \tag{13.19}$$

This is referred to as *orthotropic* symmetry.

(iii) Transversely Isotropic Symmetry

For symmetry with respect to a 90° rotation about one axis, say the x_3-axis, it can be shown [using relation (13.12)] that σ_{ij} has 2 independent components:

$$\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{11} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}. \tag{13.20}$$

This is referred to as *transversely isotropic* symmetry. Note that *crystals* with a 6-fold rotational symmetry axis (hexagonal), a 4-fold rotational symmetry axis (tetragonal), or a 3-fold rotational symmetry axis (trigonal) are all transversely isotropic with respect to the conductivity (Nye 1957). (However, neither a tetragonal nor a trigonal crystal has elastic transverse isotropy; see Section 13.3.2.) A crystal has n-fold rotational symmetry if the crystal appears unchanged when it is rotated about an axis through $2\pi/n$ radians, where n is a positive integer.

(iv) Isotropic Symmetry

When the conductivity is independent of the orientation of the coordinate system, it can be shown [using relation (13.12)] that σ_{ij} has only one independent component:

$$\begin{bmatrix} \sigma & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & \sigma \end{bmatrix}. \tag{13.21}$$

This is referred to as *isotropic* symmetry. Note that the conductivity tensor of a cubic crystal (i.e., one that has four 3-fold rotation axes) is isotropic.

If the material is isotropic in d dimensions, then the conductivity tensor is specified by the scalar σ, i.e,

$$\boldsymbol{\sigma} = \sigma \boldsymbol{I}, \tag{13.22}$$
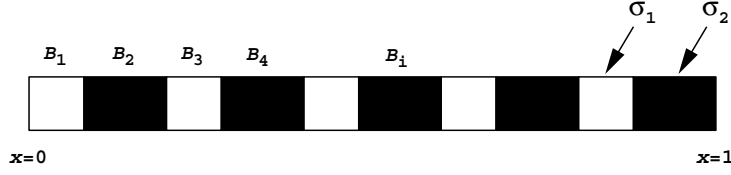
where

Figure 13.3 One-dimensional periodic composite. The white and shaded regions have conductivities σ_1 and σ_2, respectively.

$$\sigma = \frac{1}{d}\text{Tr}\ \boldsymbol{\sigma} = \frac{1}{d}\boldsymbol{\sigma} : \boldsymbol{I} \qquad (13.23)$$

and $\text{Tr}\ \boldsymbol{a} \equiv \boldsymbol{a} : \boldsymbol{I} = a_{ii}$ indicates the trace of a second-order tensor $\boldsymbol{a}$.

13.2.3 Model One-Dimensional Problem

It is instructive to consider a simple one-dimensional periodic composite model (depicted in Figure 13.3) as a prelude to the homogenization of arbitrary periodic media in any dimension. The following example is an adaptation of one given by Persson, Persson, Svanstedt and Wyller (1989). Let the composite consist of a periodic arrangement of two phases with volume fractions ϕ_1 and ϕ_2 in the interval $[0, 1]$. Phase 1 lies in regions $B_1, B_3, \ldots, B_{n-1}$, and phase 2 lies in regions $B_2, B_4, \ldots, B_n$, where n is even. The fineness of the microstructure can be adjusted by varying the number of periodic unit (i.e., repeating) cells $m = n/2$. Let us subject the end $x = 0$ to a unit flux and the opposite end $x = 1$ to a potential (temperature) $T = 0$. Therefore, the potential (temperature) profile in the bar is governed by

$$-\frac{d}{dx}\left[\sigma(x)\frac{dT}{dx}\right] = 0$$

subject to the boundary conditions

$$-\sigma_1 \frac{dT}{dx}\bigg|_{x=0} = 1, \qquad T(1) = 0.$$

According to the discussion of Section 13.2.1, this problem can be reformulated as

$$\frac{d^2 T}{dx^2} = 0, \qquad \text{in } B_i, \quad i = 1, \ldots, n,$$

$$\left.\begin{array}{c} \sigma^+(x)\dfrac{dT^+(x)}{dx} = \sigma^-(x)\dfrac{dT^-(x)}{dx} \\[2mm] T^+(x) = T^-(x) \end{array}\right\} \text{ on all interfaces,}$$

with the aforementioned boundary conditions, and where the superscripts $+$ and $-$ on a function denote its limits from the right and left, respectively. The potential $T(x)$ can be written as
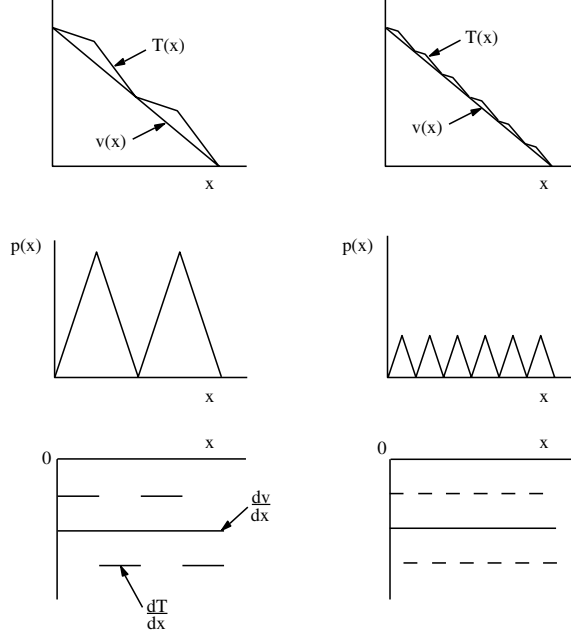
Figure 13.4   The functions $T(x)$, $v(x)$, and $p(x)$ and derivatives dT/dx and dv/dx for $n = 4$ (left panel) and $n = 10$ (right panel) when $\sigma_1 \geq \sigma_2$ and $\phi_1 = \phi_2 = 0.5$.

$$T(x) = v(x) + p(x),$$

where $p(x)$ is a *periodic function* and $v(x)$ is a linear function obeying the boundary value problem

$$\frac{d^2v}{dx^2} = 0 \qquad \text{for all } x,$$

$$-\sigma_e \left.\frac{dv}{dx}\right|_{x=0} = 1, \qquad v(1) = 0,$$

and the effective conductivity σ_e is given by the harmonic mean of the phase conductivities, i.e.,

$$\sigma_e = \langle \sigma^{-1} \rangle^{-1} = \left(\frac{\phi_1}{\sigma_1} + \frac{\phi_2}{\sigma_2} \right)^{-1}. \tag{13.24}$$

Remarks:
1. It will be shown in Chapter 16 that the harmonic average expression (13.24) is also the correct result for arbitrary random one-dimensional media.
2. It is expected that $p(x)$ converges to zero and, hence, that $T(x)$ converges uniformly to $v(x)$ as $n \to \infty$. Note that while the derivative dT/dx does not converge to dv/dx, the derivatives converge in the *weak* sense; i.e., the average of dT/dx over the domain converges to dv/dx as $n \to \infty$. Figure 13.4 shows the afore-
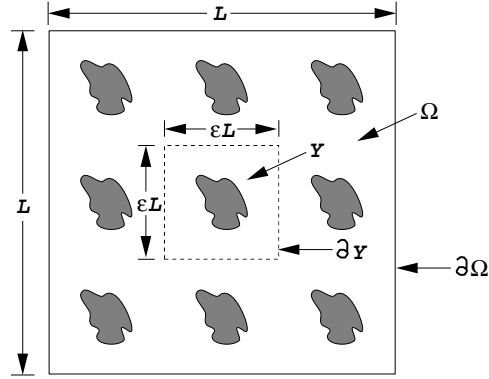
Figure 13.5 Two-dimensional periodic medium with square cells in a domain Ω with boundary $\partial\Omega$. The volume of the domain is L^2. The unit cell Y has a side of length ϵL, where $\epsilon = 1/3$, with a boundary ∂Y.

mentioned quantities plotted for the cases $n = 4$ and $n = 10$ with $\sigma_1 \geq \sigma_2$ and $\phi_1 = \phi_2 = 0.5$.

13.2.4 Homogenization of Periodic Problem in $\Re^d$

Consider now the homogenization problem for a periodic medium contained in some region Ω in $\Re^d$ with a piecewise smooth boundary $\partial\Omega$ (see Figure 13.5). The treatment given here is based on the works of Bensoussan et al. (1978) and Sanchez-Palencia (1980).

Consider an *arbitrary* periodic conductivity tensor $\boldsymbol{\sigma}(\boldsymbol{x})$ and introduce $\epsilon \geq 0$ as a parameter for varying the period by defining $\boldsymbol{\sigma}^\epsilon(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{y})$, where $\boldsymbol{y}$ is the fast variable

$$y = \frac{x}{\epsilon}. \tag{13.25}$$

We define a *Y-periodic* function $\boldsymbol{F}(\boldsymbol{y})$ to be one that is periodic in $\boldsymbol{y}$ over some *unit cell* Y. Thus, $\boldsymbol{\sigma}(\boldsymbol{y})$ is a Y-periodic function. To indicate that the local temperature depends on ϵ, we write $T^\epsilon(\boldsymbol{x}) = T(\boldsymbol{x}, \boldsymbol{y})$, where $\boldsymbol{x}$ on the *right side* signifies the slow variable. Also, we allow for a source term $f(\boldsymbol{x})$, which just depends on the slow variable. Thus, the governing equations are

$$-\frac{\partial}{\partial x_i}\left[\sigma_{ij}^\epsilon(\boldsymbol{x})\frac{\partial T^\epsilon}{\partial x_j}\right] = f(\boldsymbol{x}) \qquad \text{in } \Omega, \tag{13.26}$$

$$T^\epsilon = c_1 \quad \text{on } \Gamma_1, \qquad -\sigma_{ij}^\epsilon\frac{\partial T^\epsilon}{\partial x_j}\, n_i = c_2 \quad \text{on } \Gamma_2, \tag{13.27}$$

where Γ_1 is a portion of the boundary $\partial\Omega$, Γ_2 is the complementary surface, n_i is the unit outward normal, and c_1 and c_2 are constants. Thus, relations (13.27) represent the general situation of mixed boundary conditions, i.e., a Dirichlet condition on Γ_1 and a Neumann condition on Γ_2.

It is natural to perform a two-scale asymptotic expansion of the solution $T^\epsilon(x)$ in terms of the global and local variables, i.e.,

$$T^\epsilon(x) = T_0(x) + \epsilon T_1(x,y) + \epsilon^2 T_2(x,y) + \cdots . \tag{13.28}$$

We remark that for any function $\Psi(x) = \Phi(x,y)$, the chain rule yields

$$\nabla\Psi = \nabla_x\Phi + \frac{1}{\epsilon}\nabla_y\Phi. \tag{13.29}$$

Substitution of the asymptotic expansion into the differential equation (13.26) yields

$$-\left[\frac{\partial}{\partial x_i} + \frac{1}{\epsilon}\frac{\partial}{\partial y_i}\right]\left[\sigma_{ij}(y)\left(\frac{\partial}{\partial x_j} + \frac{1}{\epsilon}\frac{\partial}{\partial y_j}\right)(T_0 + \epsilon T_1 + \epsilon^2 T_2 + \cdots)\right]$$
$$= [\epsilon^{-2}A_0 + \epsilon^{-1}A_1 + A_2][T_0 + \epsilon T_1 + \epsilon^2 T_2 + \cdots] = f, \tag{13.30}$$

where the differential operators A_0, A_1, and A_2 are given by

$$A_0 = -\frac{\partial}{\partial y_i}\left[\sigma_{ij}(y)\frac{\partial}{\partial y_j}\right], \qquad A_1 = -\frac{\partial}{\partial y_i}\left[\sigma_{ij}(y)\frac{\partial}{\partial x_j}\right] - \sigma_{ij}(y)\frac{\partial^2}{\partial x_i\partial y_j},$$

$$A_2 = -\sigma_{ij}(y)\frac{\partial^2}{\partial x_i x_j}.$$

Equating powers of ϵ leads to the following three lowest-order equations:

$$A_0 T_0 = 0, \tag{13.31}$$

$$A_0 T_1 + A_1 T_0 = 0, \tag{13.32}$$

$$A_0 T_2 + A_1 T_1 + A_2 T_0 = f. \tag{13.33}$$

Before stating a very useful theorem, we must first introduce a definition. The spatial average of a Y-periodic function $F(y)$ over the unit cell Y, denoted by $\langle F(y)\rangle$, is defined by

$$\langle F\rangle \equiv \frac{1}{|Y|}\int_Y F(y)dy, \tag{13.34}$$

where $|Y|$ is the d-dimensional volume (measure) of Y. The quantity $F(y)$ may represent a tensor of arbitrary order.

Theorem 13.1
Let $F(y)$ be a Y-periodic function that is square integrable. For the boundary value problem

$$A_0\Phi(y) = F(y) \quad in~Y, \tag{13.35}$$

where $\Phi(y)$ is Y-periodic, the following hold:

(i) There exists a solution Φ if and only if $\langle F(y)\rangle = 0$.
(ii) If a solution exists, it is unique up to an additive constant.

The proof of this theorem may be found in Bensoussan et al. (1978).

The function $T_0(x)$ automatically satisfies $A_0 T_0 = 0$. Equation (13.32) can be expressed as

$$A_0 T_1 = \frac{\partial \sigma_{ij}}{\partial y_i} \frac{\partial T_0}{\partial x_j},$$

where x is just a parameter here. Now consider the "cell problem"

$$A_0 \chi_j = \frac{\partial \sigma_{ij}}{\partial y_i} \quad \text{in } Y, \tag{13.36}$$

where the function $\chi_j(y)$ is Y-periodic. Gauss's divergence theorem gives

$$\int_Y \frac{\partial \sigma_{ij}}{\partial y_i} dy = \int_{\partial Y} \sigma_{ij} n_i dS = 0, \tag{13.37}$$

where ∂Y is the boundary of the unit cell. Periodicity of σ renders the surface integral to be zero. Thus, by invoking Theorem 13.1, we get the solution of equation (13.32) as

$$T_1(x, y) = \chi_j(y) \frac{\partial T_0}{\partial x_j} + u(x), \tag{13.38}$$

where $\chi_j(y)$ is a solution of (13.36), unique up to a function $u(x)$ that depends on x only. By using the same theorem once more, we find that (13.33) has a Y-periodic solution T_2 if and only if

$$\langle f - A_1 T_1 - A_2 T_0 \rangle = 0,$$

or, equivalently,

$$\frac{1}{Y} \int_Y \left[f - \frac{\partial(\sigma_{ik} \chi_j)}{\partial y_k} \frac{\partial^2 T_0}{\partial x_i x_j} + \frac{\partial \sigma_{ij}}{\partial y_i} \frac{\partial u}{\partial x_j} - \sigma_{ik} \frac{\partial \chi_j}{\partial y_k} \frac{\partial^2 T_0}{\partial x_i \partial x_j} + \sigma_{ij} \frac{\partial^2 T_0}{\partial x_i \partial x_j} \right] dy = 0.$$

The functions σ_{ij} and χ_j are Y-periodic, and the functions T_0 and u are independent of y. Therefore, the second and third terms in the integral immediately above vanish by Gauss's divergence theorem, and the integral simplifies to

$$- (\sigma_e)_{ij} \frac{\partial^2 T_0}{\partial x_i \partial x_j} = f, \tag{13.39}$$

where

$$(\sigma_e)_{ij} = \langle \sigma_{ij} \rangle + \left\langle \sigma_{ik} \frac{\partial \chi_j}{\partial y_k} \right\rangle. \tag{13.40}$$

The relations (13.39) and (13.40) are the key results: They show that the heterogeneous periodic medium will behave like a homogeneous medium, governed by the steady-state conduction equation (13.39), with a constant conductivity tensor σ_e in the limit $\epsilon \to 0$. This is tantamount to the specification of an averaged Ohm's (Fourier's) law, i.e.,

$$\langle \boldsymbol{J}(\boldsymbol{x}) \rangle = \sigma_e \cdot \langle \boldsymbol{E}(\boldsymbol{x}) \rangle, \tag{13.41}$$

where σ_e is given precisely by (13.40). This relation is easily obtained by taking the gradient of expansion (13.28), computing the local fields $\boldsymbol{E}$ and $\boldsymbol{J}$ using definitions (13.5) and (13.6), respectively, averaging the local fields, and utilizing the fact that the periodicity of χ renders $\langle \nabla \chi \rangle = 0$. In the limit that $\epsilon \to 0$, one finally gets the averaged relation (13.41). [The precise manner in which the local fields converge to the homogenized fields in the limit $\epsilon \to 0$ has been investigated by Bensoussan et al. (1978) and Sanchez-Palencia (1980).] The above analysis could also be applied to the situation in which the local conductivity $\sigma(\boldsymbol{x}, \boldsymbol{y})$ depends on the slow and fast variables $\boldsymbol{x}, \boldsymbol{y}$, leading to an effective conductivity σ_e that varies on macroscopic length scales.

13.2.5 Homogenization of Random Problem in $\Re^d$

The analogue of periodicity in the random setting is statistical homogeneity and ergodicity. Each realization ω of the random medium of space $\mathcal{V} \in \Re^d$ is partitioned into two random sets, or phases, as described in Section 13.1 (see Figure 13.2). Let $\sigma^\epsilon(\boldsymbol{x}) = \sigma(\boldsymbol{y}; \omega)$ be the symmetric conductivity tensor, where $\boldsymbol{y} = \boldsymbol{x}/\epsilon$ is the fast variable associated with the microstructure. The conductivity $\sigma(\boldsymbol{y}; \omega)$ is a *statistically homogeneous function* (in the strict sense defined in Section 2.2.2) that is *positive definite* and *bounded*. The temperature distribution $T^\epsilon(\boldsymbol{x}) = T(\boldsymbol{x}, \boldsymbol{y}; \omega)$ satisfies

$$-\frac{\partial}{\partial x_i} \left[\sigma_{ij}^\epsilon(\boldsymbol{x}) \frac{\partial T^\epsilon}{\partial x_j} \right] = f(\boldsymbol{x}) \qquad \text{in } \mathcal{V} \tag{13.42}$$

for each realization of the ensemble, and we assume that $T^\epsilon = 0$ is specified on the boundary of $\mathcal{V}$. Ultimately, we consider the limit that the volume $V \to \infty$ such that the volume fraction remains fixed, and then we invoke the ergodic hypothesis, i.e., we study *ergodic media*.

The problem now is to analyze the behavior of $T^\epsilon(\boldsymbol{x})$ as $\epsilon \to 0$. Papanicolaou and Varadan (1979) have shown that when σ_{ij}^ϵ is statistically homogeneous and ergodic, there exists an effective conductivity tensor $(\sigma_e)_{ij}$, independent of the boundary conditions in the infinite-volume limit (Papanicolaou and Varadan 1979, Golden and Papanicolaou 1983), such that if $T_0(\boldsymbol{x})$ is the solution of the *deterministic* heat equation

$$-(\sigma_e)_{ij} \frac{\partial^2 T_0}{\partial x_i \partial x_j} = f(\boldsymbol{x}), \tag{13.43}$$

then

$$\int_{\mathcal{V}} \langle |T^\epsilon(\boldsymbol{x}) - T_0(\boldsymbol{x})|^2 \rangle \, d\boldsymbol{x} \to 0, \quad \text{as } \epsilon \to 0. \tag{13.44}$$

Thus, an ergodic heterogeneous medium will behave like a homogeneous deterministic medium with conductivity tensor $(\sigma_e)_{ij}$ when ϵ becomes very small. The result (13.43) is identical in form to result (13.39) for the periodic medium.

To prove the above statement, one again assumes a two-scale asymptotic expansion of $T^\epsilon(\boldsymbol{x}; \omega)$ of the type

$$T^\epsilon(\boldsymbol{x}; \omega) = T_0(\boldsymbol{x}) + \epsilon T_1(\boldsymbol{x}, \boldsymbol{y}; \omega) + \epsilon^2 T_2(\boldsymbol{x}, \boldsymbol{y}; \omega) + \cdots, \tag{13.45}$$

which is substituted into the governing equation (13.42). Since the procedure is similar to the one used for periodic media, the details are not given here, except to say that in the end we find that the effective conductivity is defined by an averaged Ohm's (Fourier's) law

$$\langle \boldsymbol{J}(\boldsymbol{x}) \rangle = \boldsymbol{\sigma}_e \cdot \langle \boldsymbol{E}(\boldsymbol{x}) \rangle, \tag{13.46}$$

where

$$(\sigma_e)_{ij} = \langle \sigma_{ij} \rangle + \left\langle \sigma_{ik} \frac{\partial \chi_j}{\partial y_k} \right\rangle, \tag{13.47}$$

the function $\chi_j(\boldsymbol{y}; \omega)$ solves

$$-\frac{\partial}{\partial y_i} \left[\sigma_{ik}(\boldsymbol{y}; \omega) \frac{\partial}{\partial y_k} \chi_j(\boldsymbol{y}; \omega) \right] = \frac{\partial}{\partial y_i} \sigma_{ij}(\boldsymbol{y}; \omega) \quad \text{in } \Re^d, \tag{13.48}$$

and angular brackets denote an *ensemble* average. Note that the definition (13.46) is consistent with the one given in Table 1.1.

Remarks:
1. There are some important differences between the random and periodic settings. In the random setting, (13.48) always has a solution χ that is not statistically homogeneous but its gradient $\nabla \chi$ is statistically homogeneous and $\langle \chi \rangle = 0$. This is to be contrasted with the periodic setting, where χ itself is a periodic solution. Furthermore, the ensemble average of the right side of (13.48) is zero by ergodicity (as detailed in many of the proofs in Chapter 14), whereas the volume average of the right side of (13.36) in the periodic case is zero by periodicity.
2. The homogenized result (13.46) for the ergodic random setting becomes identical in form to the corresponding periodic result (13.41) in the limit $\epsilon \to 0$ when angular brackets are interpreted as ensemble averages.
3. Macroscopic variation of the effective conductivity tensor could be allowed for, i.e., $\boldsymbol{\sigma}_e(\boldsymbol{x})$ may be assumed to depend on the position $\boldsymbol{x}$, provided that the length scales associated with such variations of $\mathcal{O}(\Lambda)$ are large enough to assume statistical homogeneity at $\boldsymbol{x}$ (local statistical homogeneity).
4. It is shown in Section 14.1.2 that $\boldsymbol{\sigma}_e$ is symmetric and positive definite if the local conductivity tensor $\boldsymbol{\sigma}$ is symmetric and positive definite.
5. In the case of conduction, *macroscopically isotropic* composites are those whose effective conductivity tensor $\boldsymbol{\sigma}_e$ is specified by the scalar σ_e, i.e.,

$$\boldsymbol{\sigma}_e = \sigma_e \boldsymbol{I}.$$

6. For composites consisting of *isotropic phases*, the following general statements can be made:

   - Statistically isotropic composites are always macroscopically isotropic composites [e.g., statistically isotropic arrays of inclusions in a matrix (see Figure 12.6)].

   - However, statistical anisotropy, as measured by correlation functions (Section 2.2.2), does not necessarily imply a *macroscopically anisotropic* composite with an effective tensor σ_e. For instance, composites with cubic symmetry are statistically anisotropic but are macroscopically isotropic (e.g., cubic lattices of spheres in a matrix).

   - Macroscopically anisotropic composites are necessarily *statistically anisotropic* [e.g., statistically anisotropic arrays of oriented cylinders or ellipsoids in a matrix (see Figure 7.1) or stratified media (see Figure 16.3)].

   Note that macroscopically anisotropic composites are not necessarily *statistically anisotropic* if some of the phases are anisotropic. For instance, systems of statistically isotropic arrays of spherical but anisotropic grains oriented in the same direction in an isotropic matrix are macroscopically anisotropic.

7. The effective relation (13.46) also applies to composites with an arbitrary number of phases that meet the standard two-scale assumption.

8. The effective conductivity tensor σ_e of a macroscopically anisotropic composite composed of M isotropic phases is a *homogeneous function of degree one* in its M scalar phase conductivities $\sigma_1, \ldots, \sigma_M$. For two isotropic phases, this means that $\sigma_e(\sigma_1, \sigma_2)$ obeys the relation

$$\boldsymbol{\sigma}_e(\alpha\sigma_1, \alpha\sigma_2) = \alpha\,\boldsymbol{\sigma}_e(\sigma_1, \sigma_2) \qquad \text{for all } \alpha. \tag{13.49}$$

   If we set the constant α equal to $1/\sigma_1$, then we get

$$\frac{\boldsymbol{\sigma}_e(\sigma_1, \sigma_2)}{\sigma_1} = \boldsymbol{\sigma}_e(1, \sigma_2/\sigma_1).$$

   Thus, the homogeneity property (13.49) enables us to reduce the independent variables from two to one (σ_2/σ_1) without any loss of generality. The homogeneity property is trivially proven using the effective relation (13.46) and the observation that $\nabla \cdot \boldsymbol{J}' = 0$ when $\boldsymbol{J}' = \alpha\boldsymbol{J}$ and $\nabla \cdot \boldsymbol{J} = 0$.

9. A given formula for the effective conductivity as a function of the phase conductivities, $\boldsymbol{\sigma}_e(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2)$, immediately gives equivalent formulas for the other class A problems by a simple replacement of the conductivities with the constants of interest. For example, letting ϵ denote the dielectric constant tensor, we can obtain an expression for the effective dielectric constant ϵ_e by the replacement $\boldsymbol{\sigma}_e \to \boldsymbol{\epsilon}_e$, $\sigma_1 \to \epsilon_1$, and $\sigma_2 \to \epsilon_2$. Similarly, for diffusion past fixed impermeable obstacles (phase 2), the

effective diffusion coefficient $\mathcal{D}_e$ is found by the replacement $\boldsymbol{\sigma}_e \to \mathcal{D}_e$, $\boldsymbol{\sigma}_1 \to \mathcal{D}_1$, and $\boldsymbol{\sigma}_2 \to \boldsymbol{0}$.

13.2.6 Frequency-Dependent Conductivity

For time-varying electric fields, such as in electromagnetic radiation, the phase conductivities and the effective conductivity $\boldsymbol{\sigma}_e$ are frequency-dependent and complex (real and imaginary parts). The optical properties of a material are often described in terms of the dielectric constant, which is also frequency-dependent and complex. The analysis is simplified if the wavelength is much larger than the heterogeneity length scale, since then Maxwell's equations of electromagnetic wave propagation reduce to the aforementioned steady-state conduction equations but with complex fields and complex properties. The reader is referred to Bergman (1978,1982) and Milton (1980, 1981a, 1981b) and references therein for pertinent literature on the subject of composites with complex properties.

13.3   Elastic Problem

In this section we discuss the local relations for the elasticity problem and elastic symmetry (Sokolnikoff 1956). The homogenized relations follow in the same way as in the previous section. We also discuss other problems that fall within class B.

13.3.1   Local Relations

For each realization ω of the random medium occupying the space $\mathcal{V} \in \Re^d$, we assume that phases 1 and 2 have constant stiffness tensors $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$, respectively. It is desired to obtain the relevant equations governing the local elastostatic fields. In what follows, we temporarily drop ω from the notation.

Local Differential Equations

Let $\boldsymbol{\tau}(\boldsymbol{x})$ and $\boldsymbol{\varepsilon}(\boldsymbol{x})$ denote respectively the symmetric local stress and strain tensors at position $\boldsymbol{x}$. Under steady state without sources, conservation of momentum requires the stress tensor $\boldsymbol{\tau}(\boldsymbol{x})$ to satisfy the equilibrium equations

$$\nabla \cdot \boldsymbol{\tau} = 0 \qquad \text{in } \mathcal{V} \tag{13.50}$$

for each realization of the ensemble. The strain field $\boldsymbol{\varepsilon}(\boldsymbol{x})$ satisfies the compatibility relations

$$\nabla \times [\nabla \times \boldsymbol{\varepsilon}]^{\mathrm{T}} = 0 \qquad \text{in } \mathcal{V}, \tag{13.51}$$

which implies the existence of a displacement field $\boldsymbol{u}$. (Here the superscript T denotes the transpose operation.) In other words, the strain can be written as a symmetrized gradient of displacements

$$\varepsilon(\boldsymbol{x}) = \frac{1}{2}\left[\nabla\boldsymbol{u}(\boldsymbol{x}) + \nabla\boldsymbol{u}(\boldsymbol{x})^{\mathrm{T}}\right]. \tag{13.52}$$

We also specify the displacement $\boldsymbol{u}$ on the boundary of $\mathcal{V}$.

Local Constitutive Relation

In order to obtain the strain field ε or displacement field $\boldsymbol{u}$ from the relations (13.50) and (13.51), we will connect $\boldsymbol{\tau}$ to ε by assuming a linear constitutive relation, i.e.,

$$\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x}) \qquad \text{in } \mathcal{V}, \tag{13.53}$$

where

$$\boldsymbol{C}(\boldsymbol{x}) = \boldsymbol{C}_1 \mathcal{I}^{(1)}(\boldsymbol{x}) + \boldsymbol{C}_2 \mathcal{I}^{(2)}(\boldsymbol{x}) \tag{13.54}$$

is the local stiffness tensor and $\mathcal{I}^{(i)}(\boldsymbol{x})$ is the indicator function for phase i, given by (2.1). Relation (13.53) is the *generalization* of Hooke's law. Here the symbol : denotes the contraction with respect to two indices. For example,

$$\boldsymbol{a} : \boldsymbol{b} = a_{ij}b_{ji}, \qquad \boldsymbol{B} : \boldsymbol{a} = B_{ijkl}a_{lk}, \tag{13.55}$$

where $\boldsymbol{a}$ and $\boldsymbol{b}$ are second-order tensors and $\boldsymbol{B}$ is a fourth-order tensor. The stress–strain relations can be expressed in inverted form

$$\varepsilon(\boldsymbol{x}) = \boldsymbol{S}(\boldsymbol{x}) : \boldsymbol{\tau}(\boldsymbol{x}), \tag{13.56}$$

where S_{ijkl} is the *compliance* tensor. The stiffness and compliance tensors are related by

$$\boldsymbol{S} : \boldsymbol{C} = \boldsymbol{I}, \tag{13.57}$$

where in component form

$$I_{ijkl} = \frac{1}{2}[\delta_{ik}\ \delta_{jl}\ +\ \delta_{il}\ \delta_{jk}] \tag{13.58}$$

is the *fourth-order identity tensor*. Note that the notation used to designate the full fourth-order identity tensor $\boldsymbol{I}$ is the same as that for the second-order identity tensor with components given by the Kronecker delta δ_{ij} (13.10). Unless otherwise noted, it will be apparent by the context whether the second- or fourth-order identity tensor is being used.

Note that (13.50), which applies anywhere in the heterogeneous material, implies that the traction vector $\boldsymbol{t} = \boldsymbol{\tau} \cdot \boldsymbol{n}$ is continuous across the interface $\partial\mathcal{V}$. Similarly, the compatibility condition (13.51) implies that the displacement $\boldsymbol{u}$ is continuous across the interface $\partial\mathcal{V}$. To summarize, the governing equations imply the *ideal* (or *perfect*) interface conditions

$$\boldsymbol{t} \text{ and } \boldsymbol{u} \text{ continuous across } \partial\mathcal{V}. \tag{13.59}$$

Computationally, the problem can be reformulated as solving (13.50)–(13.53) in *each phase* subject to the interface conditions (13.59) and boundary conditions on the macroscopic sample surface. Imperfect interfaces (where the displacement $\boldsymbol{u}$ jumps across

the interface, due to debonding, and/or t jumps across the interface) were noted in Chapter 1.

That C_{ijkl} (S_{ijkl}) is a fourth-order tensor can be demonstrated by showing that its d^4 components in d dimensions, referred to a coordinate system, transform to d^4 components in another "primed" coordinate system according to the transformation rule for fourth-order tensors, i.e.,

$$C'_{ijkl} = l_{im}l_{jn}l_{kp}l_{lq}\, C_{mnpq}. \tag{13.60}$$

Here l_{ij} are the aforementioned direction cosines.

Now, since the stress tensor is symmetric (i.e., $\tau_{ij} = \tau_{ji}$), we must have

$$C_{ijkl} = C_{jikl}. \tag{13.61}$$

Also, since the strain tensor ε_{ij} is symmetric, then

$$C_{ijkl} = C_{ijlk}. \tag{13.62}$$

These two conditions enable one to reduce the 81 independent components of C_{ijkl} to 36 for three-dimensional elasticity. In d dimensions, the d^4 independent components are reduced to $[d(d+1)/2]^2$ components.

When the stress can be expressed as a derivative of the *strain energy density function* u with respect to strain such that

$$\tau_{ij} = \frac{\partial u}{\partial \varepsilon_{ij}}, \tag{13.63}$$

then it immediately follows from the linear Hooke's law (13.53) that u, up to an additive constant, is given by

$$u = \frac{1}{2}\tau_{ij}\varepsilon_{ij} = \frac{1}{2}\varepsilon_{kl}C_{ijkl}\varepsilon_{ij} \geq 0, \tag{13.64}$$

and hence the stiffness tensor must additionally have the symmetry

$$C_{ijkl} = C_{klij}. \tag{13.65}$$

(The scalar quantity u should not be confused with the vector displacement $\boldsymbol{u}$.) In d dimensions, condition (13.65) further reduces the number of independent elastic constants to $d(d+1)(d^2+d+2)/8$. For $d = 3$, this means that the number of independent elastic constants is reduced to 21. From relations (13.57) and (13.61)–(13.65), we see that the compliance tensor S_{ijkl} must possess the same symmetries as the stiffness tensor C_{ijkl}.

Note that the nonnegativity of the strain energy density function u [cf. (13.64)] places restrictions on the components of $\boldsymbol{C}$ and implies that the stiffness tensor $\boldsymbol{C}$ (or compliance tensor $\boldsymbol{S}$) is *positive definite*. Recall that a symmetric fourth-order tensor $\boldsymbol{A}$ (A_{ijkl}) is *positive semidefinite*, if for any second-order tensor $\boldsymbol{b}$ (b_{ij}) in $\Re^d$,

$$b_{ij}A_{ijkl}b_{kl} \geq 0. \tag{13.66}$$

If only the inequality of (13.66) applies for any nonzero tensor $b \neq 0$, then A is said to be positive definite. Since the equality of (13.64) holds only for $\varepsilon = 0$, C is positive definite, and therefore is also positive semidefinite. (Any positive definite tensor A is also positive semidefinite, since either $b \neq 0$ or $b = 0$.) Note that for C and S to be positive definite, it is necessary and sufficient that their $d(d + 1)/2$ real eigenvalues be positive.

In summary, the number of independent elastic constants for the general anisotropic linearly elastic material is reduced to 21 for three-dimensional elasticity. Moreover, if certain elastic symmetries exist in the material, this number will be reduced even further, as discussed below.

13.3.2 Elastic Symmetry

Elastic symmetry is expressed by the property that the coefficients $C_{ijkl}(S_{ijkl})$ remain invariant under certain transformations of the coordinates. As in the previous section, basic coordinate changes are (a) reflection in a plane, (b) rotation about an axis, and (c) rotation about an axis combined with reflection in a plane that is normal to the axis.

Consider a linearly elastic homogeneous material. We restrict ourselves initially to three dimensions. In light of the symmetry relations (13.61), (13.62), and (13.65), the generalized Hooke's law (13.53) really represents only six independent equations with 21 elastic constants. This is conveniently represented as a matrix equation expressing a six-element column vector of stresses in terms of a six-element column vector of strains. We write

$$
\begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \\ \tau_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}, \tag{13.67}
$$

where the elements of the two column vectors τ_i and ε_i are

$$
\tau_1 = \tau_{11}, \ \tau_2 = \tau_{22}, \ \tau_3 = \tau_{33}, \ \tau_4 = \tau_{23}, \ \tau_5 = \tau_{13}, \ \tau_6 = \tau_{12},
$$

$$
\varepsilon_1 = \varepsilon_{11}, \ \varepsilon_2 = \varepsilon_{22}, \ \varepsilon_3 = \varepsilon_{33}, \ \varepsilon_4 = 2\varepsilon_{23}, \ \varepsilon_5 = 2\varepsilon_{13}, \ \varepsilon_6 = 2\varepsilon_{12}.
$$

The matrix equation (13.67) can be written more compactly as

$$
\tau_i = C_{ij}\varepsilon_j, \tag{13.68}
$$

where C_{ij} is the 6×6 symmetric matrix whose elements are given in (13.67). The mapping between the tensor C_{ijkl} and the matrix C_{pq} is accomplished by replacing the subscripts ij (or kl) by p (or q) using the following rules:

$$
11 \leftrightarrow 1, \ 22 \leftrightarrow 2, \ 33 \leftrightarrow 3, \ 23 \text{ or } 32 \leftrightarrow 4, \ 13 \text{ or } 31 \leftrightarrow 5, \ 12 \text{ or } 21 \leftrightarrow 6.
$$

The relation (13.68) may be inverted to give

$$\varepsilon_i = S_{ij}\tau_j, \tag{13.69}$$

where the 6×6 symmetric matrix S_{ij} is just the inverse of the matrix C_{ij} given in (13.68). The transformation between the tensor S_{ijkl} and the matrix S_{pq} is similar to that between C_{ijkl} and C_{pq} except for the following conditions: $S_{pq} = S_{ijkl}$ if $1 \le p, q \le 3$; $S_{pq} = 2S_{ijkl}$ if $1 \le p \le 3$ and $4 \le q \le 6$ or if $4 \le p \le 6$ and $1 \le q \le 3$; $S_{pq} = 4S_{ijkl}$ if $4 \le p, q \le 6$. It is noteworthy that the matrices C_{ij} and S_{ij} do not transform as tensors.

In what follows we consider a number of different cases where the tensor C_{ijkl} (S_{ijkl}) remains invariant to certain transformations according to the rule (13.60). We then represent the elastic symmetry class as a 6×6 stiffness or compliance matrix.

(i) Monoclinic Symmetry

For symmetry with respect to one plane, say the x_1-x_2 plane, it can be shown that C_{ij} has 13 independent components:

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & C_{45} & 0 \\ 0 & 0 & 0 & C_{45} & C_{55} & 0 \\ C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66} \end{bmatrix}. \tag{13.70}$$

This is referred to as *monoclinic* symmetry. As in the general anisotropic case, here a pure shear strain can give rise to a normal stress.

(ii) Orthotropic Symmetry

For symmetry with respect to three orthogonal planes, it can be shown that C_{ij} has 9 independent components:

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}. \tag{13.71}$$

This is referred to as *orthotropic* symmetry.

(iii) Transverse Square Symmetry

For symmetry with respect to a $90°$ rotation about one axis, say the x_1-axis, it can be shown that C_{ij} has 6 independent components:

$$
\boldsymbol{C} = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{12} & C_{23} & C_{22} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{66} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}. \tag{13.72}
$$

This is referred to as *transverse square* symmetry. A tetragonal crystal has such symmetry.

(iv) Transversely Isotropic Symmetry

For symmetry of rotation with respect to one axis, say the x_1-axis, it is easily shown that C_{ij} has 5 independent components:

$$
\boldsymbol{C} = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{12} & C_{23} & C_{22} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2}(C_{22} - C_{23}) & 0 & 0 \\
0 & 0 & 0 & 0 & C_{66} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}. \tag{13.73}
$$

This is referred to as *transversely isotropic* symmetry. A crystal with a 6-fold rotational symmetry axis (hexagonal) is transversely isotropic with respect to the stiffness (Nye 1957). Although a crystal with a 3-fold rotational symmetry axis (trigonal) is not transversely isotropic (Nye 1957), there are only two independent elastic moduli in the transverse plane. Hence, *two-dimensional* crystals with a 3-fold rotational symmetry axis are elastically isotropic.

It is useful to explicitly write the stress–strain relations here, since the case of transverse isotropy is treated in some detail in subsequent portions of the book. Given C_{ij} above, it follows that

$$
\begin{aligned}
\tau_{11} &= C_{11}\varepsilon_{11} + C_{12}\varepsilon_{22} + C_{12}\varepsilon_{33}, \\
\tau_{22} &= C_{12}\varepsilon_{11} + C_{22}\varepsilon_{22} + C_{23}\varepsilon_{33}, \\
\tau_{33} &= C_{12}\varepsilon_{11} + C_{23}\varepsilon_{22} + C_{22}\varepsilon_{33}, \\
\tau_{23} &= (C_{22} - C_{23})\varepsilon_{23}, \\
\tau_{13} &= 2C_{66}\varepsilon_{13}, \\
\tau_{12} &= 2C_{66}\varepsilon_{12}.
\end{aligned} \tag{13.74}
$$

It is convenient to relate the five constants C_{11}, C_{12}, C_{22}, C_{23}, and C_{66} to more easily measurable *engineering* elastic moduli, such as Young's modulus, Poisson's ratios, and the shear modulus. First consider applying a uniform strain ε in both the x_2-direction and x_3-direction such that axial extension in the x_1-direction is prohibited, i.e.,

$$\varepsilon_{11} = 0, \quad \varepsilon_{22} = \varepsilon_{33} = \varepsilon.$$

Letting

$$\tau_{22} = \tau_{33} = \tau,$$

we find from (13.75) that

$$\tau = 2k_{23}\varepsilon,$$

where

$$k_{23} = \frac{1}{2}(C_{22} + C_{33}) \tag{13.75}$$

is the *plane strain* or *transverse* bulk modulus.

Now consider a simple state of uniaxial stress, i.e.,

$$\tau_{11} \neq 0, \quad \tau_{22} = \tau_{33} = \tau_{12} = \tau_{23} = \tau_{13} = 0.$$

For such a state, (13.75) reveals that

$$\tau_{11} = E_{11}\varepsilon_{11},$$

where

$$E_{11} = C_{11} - \frac{2C_{12}^2}{C_{22} + C_{33}} \tag{13.76}$$

is the *longitudinal* Young's modulus. The Poisson ratios that characterize the typical lateral contraction (expansion) that accompanies uniaxial tension (compression) in the x_1-direction are defined by the relations

$$v_{12} = -\frac{\varepsilon_{22}}{\varepsilon_{11}}, \qquad v_{13} = -\frac{\varepsilon_{33}}{\varepsilon_{11}}.$$

Generally, v_{ij} is Poisson's ratio, where the first index i indicates the direction of the imposed stress or strain and the second index j indicates the response direction. For the aforementioned uniaxial stress state, we have from (13.75) that

$$v_{12} = v_{13} = \frac{C_{12}}{C_{22} + C_{33}}. \tag{13.77}$$

The directly measurable shear moduli are defined in the usual way, i.e.,

$$G_{12} = G_{13} = C_{66}, \tag{13.78}$$

$$G_{23} = \frac{1}{2}(C_{22} - C_{33}). \tag{13.79}$$

Using the relations above, we can express the five coefficients of (13.73) in terms of the directly measurable moduli:

$$C_{11} = E_{11} + 4v_{12}^2 k_{23}, \qquad C_{12} = 2k_{23}v_{12},$$
$$C_{22} = k_{23} + G_{23}, \qquad C_{23} = k_{23} - G_{23}, \qquad C_{66} = G_{12}.$$

Other engineering moduli could have been measured. For example, for a state of uniaxial stress in the x_2-direction, one would measure E_{22}, ν_{21} ($\neq \nu_{12}$), and ν_{23}, and for uniaxial stress in the x_3-direction, one would measure E_{33}, ν_{31} ($\neq \nu_{13}$), and ν_{32}. Now, since some of these moduli are equal by symmetry, we will henceforth use the following notation:

$$E^L \equiv E_{11}, \quad \nu^L \equiv \nu_{12} = \nu_{13}, \quad G^L \equiv G_{12} = G_{13}, \tag{13.80}$$

$$E^T \equiv E_{22} = E_{33}, \quad \nu^T \equiv \nu_{23} = \nu_{32}, \quad G^T \equiv G_{23}, \quad k^T \equiv k_{23}. \tag{13.81}$$

Here E^L, ν^L, and G^L are the longitudinal Young modulus, Poisson ratio, and shear modulus, respectively, whereas E^T, ν^T, G^T, and k^T are the transverse Young modulus, Poisson ratio, shear modulus, and bulk modulus, respectively.

Since there are only five independent moduli, there are interrelations among the properties. For example, two of them are

$$G^T = \frac{E^T}{2(1 + \nu^T)} \tag{13.82}$$

and

$$\frac{4}{E^T} = \frac{1}{k^T} + \frac{1}{G^T} + \frac{4(\nu^L)^2}{E^L}. \tag{13.83}$$

The previous two relations can be combined to give the following relation for the transverse Poisson ratio ν^T:

$$\nu^T = \frac{k^T - G^T - 4k^T G^T (\nu^L)^2 / E^L}{k^T + G^T + 4k^T G^T (\nu^L)^2 / E^L}. \tag{13.84}$$

Other property interrelations have been given by Christensen (1979).

The nonnegativity of the strain energy density function u [cf. (13.64)], implies that the moduli k^T, G^T, and E^L are all positive. Using these nonnegativity conditions and (13.84), it is easily shown that

$$-1 \leq \nu^T \leq 1. \tag{13.85}$$

Note that the transverse Poisson ratio can be negative, with -1 being the lower limit. A negative Poisson's ratio implies that a uniaxial tensile (compressive) load applied in any direction in the transverse plane will lead to an expansion (contraction) of the material in the direction orthogonal to the applied load. The lower limit of -1 is found by taking the limit $G^T/k^T \to \infty$ and $E^L/G^T \to \infty$. The upper limit of 1 is obtained by taking the limit that $k^T/G^T \to \infty$ and $E^L/k^T \to \infty$. By contrast, for a three-dimensional isotropic material, Poisson's ratio must lie in the interval $[-1, 0.5]$, as shown below. It is interesting to note that in the limit $E^L/(\nu^L)^2 \to \infty$, (13.83) and (13.84) respectively reduce to

$$4/E^T = 1/k^T + 1/G^T, \quad \nu^T = (k^T - G^T)/(k^T + G^T),$$

which are the same as the *two-dimensional isotropic elasticity* results, given by (13.103) and (13.104) with $d = 2$.

We can express the aforementioned results for transverse isotropy in terms of the 6×6 compliance matrix S_{ij} as follows:

$$
S = \begin{bmatrix}
\dfrac{1}{E^L} & -\dfrac{\nu^L}{E^L} & -\dfrac{\nu^L}{E^L} & 0 & 0 & 0 \\[2mm]
-\dfrac{\nu^L}{E^L} & \dfrac{1}{E^T} & -\dfrac{\nu^T}{E^T} & 0 & 0 & 0 \\[2mm]
-\dfrac{\nu^L}{E^L} & -\dfrac{\nu^T}{E^T} & \dfrac{1}{E^T} & 0 & 0 & 0 \\[2mm]
0 & 0 & 0 & \dfrac{1}{G^T} & 0 & 0 \\[2mm]
0 & 0 & 0 & 0 & \dfrac{1}{G^L} & 0 \\[2mm]
0 & 0 & 0 & 0 & 0 & \dfrac{1}{G^L}
\end{bmatrix}.
\tag{13.86}
$$

(v) Cubic Symmetry

For symmetry with respect to $90°$ rotations about two perpendicular axes, say the x_1-axis and x_2-axis, it can be shown that C_{ij} has 3 independent components:

$$
C = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix}.
\tag{13.87}
$$

This is referred to as *cubic* symmetry.

(vi) Isotropic Symmetry

When the elastic moduli are independent of the orientation of the coordinate system, there are two independent elastic moduli:

$$
C = \begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & \tfrac{1}{2}(C_{11} - C_{12}) & 0 & 0 \\
0 & 0 & 0 & 0 & \tfrac{1}{2}(C_{11} - C_{12}) & 0 \\
0 & 0 & 0 & 0 & 0 & \tfrac{1}{2}(C_{11} - C_{12})
\end{bmatrix}.
\tag{13.88}
$$

This is referred to as *isotropic* symmetry. The elastic constants C_{12} and $(C_{11} - C_{12})$ are identified as the Lamé constant λ and shear modulus G, i.e.,

$$C_{12} = \lambda, \qquad \frac{1}{2}(C_{11} - C_{12}) = G, \qquad C_{11} = \lambda + 2G.$$

In indicial notation, the stress–strain relations for a d-dimensional material are written as

$$\tau_{ij} = \lambda \varepsilon_{kk}\, \delta_{ij} + 2G\varepsilon_{ij}, \qquad i,j = 1,\ldots,d. \tag{13.89}$$

The strain–stress relation can be written as

$$\varepsilon_{ij} = -\frac{\nu}{E}\, \tau_{kk}\, \delta_{ij} + \frac{1+\nu}{E}\tau_{ij}, \qquad i,j = 1,\ldots,d, \tag{13.90}$$

where E is Young's modulus (uniaxial stress in any direction divided by the strain in the same direction) and ν is Poisson's ratio (negative of the strain in the direction of a uniaxial stress divided by the associated transverse strain).

Alternatively, the stress–strain relations can be represented in terms of the *deviatoric* and *dilatational* (hydrostatic) components of the stress and strain. Let s_{ij} and e_{ij} be the deviatoric components of stress and strain, defined in any space dimension d as

$$s_{ij} = \tau_{ij} - \frac{1}{d}\, \delta_{ij}\, \tau_{kk}, \tag{13.91}$$

$$e_{ij} = \varepsilon_{ij} - \frac{1}{d}\, \delta_{ij}\varepsilon_{kk}. \tag{13.92}$$

Thus, we have from (13.89) that

$$\begin{aligned} s_{ij} &= 2Ge_{ij}, &&\text{(deviatoric relation)},\\ \tau_{kk} &= dK\varepsilon_{kk}, &&\text{(dilatational relation)}, \end{aligned} \tag{13.93}$$

where K is the bulk modulus governing volumetric or dilatational changes, which can be expressed in terms of λ and G as

$$K = \lambda + \frac{2}{d}G. \tag{13.94}$$

The nonnegativity of the strain energy density function u [cf. (13.64)] implies that the moduli K, G, and E are all positive.

For subsequent discussion it will be convenient to obtain the appropriate form of the fourth-order tensors C_{ijkl} and S_{ijkl} for the isotropic case. It is seen from the stress–strain relation (13.89) that the stiffness tensor can be written in terms of the projection tensors $\boldsymbol{\Lambda}_h$ and $\boldsymbol{\Lambda}_s$ as follows:

$$\boldsymbol{C} = dK\boldsymbol{\Lambda}_h + 2G\boldsymbol{\Lambda}_s, \tag{13.95}$$

where, in component form,

$$(\Lambda_h)_{ijkl} = \frac{1}{d}\delta_{ij}\delta_{kl}, \tag{13.96}$$

$$(\Lambda_s)_{ijkl} = \frac{1}{2}[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] - \frac{1}{d}\delta_{ij}\delta_{kl}. \tag{13.97}$$

The tensor $\mathbf{\Lambda}_h$ projects onto fields that are everywhere isotropic, i.e., hydrostatic fields, whereas the tensor $\mathbf{\Lambda}_s$ projects onto fields that are everywhere trace-free, i.e., shear fields. We note the following useful identities:

$$(\Lambda_h)_{ijkl}I_{ijkl} = 1, \qquad (\Lambda_s)_{ijkl}I_{ijkl} = \frac{(d-1)(d+2)}{2},$$

$$(\Lambda_h)_{ijkl} + (\Lambda_s)_{ijkl} = I_{ijkl}, \qquad (\Lambda_h)_{ijmn}(\Lambda_h)_{mnkl} = (\Lambda_h)_{ijkl}, \qquad (13.98)$$

$$(\Lambda_s)_{ijmn}(\Lambda_s)_{mnkl} = (\Lambda_s)_{ijkl}, \qquad (\Lambda_h)_{ijmn}(\Lambda_s)_{mnkl} = 0.$$

Similarly, the strain–stress relations (13.90) give the compliance tensor S as

$$S = \frac{1 + v(1-d)}{E}\mathbf{\Lambda}_h + \frac{1+v}{E}\mathbf{\Lambda}_s. \qquad (13.99)$$

Taking the inverse of relation (13.95) and using the identities (13.98) yields

$$S = \frac{1}{dK}\mathbf{\Lambda}_h + \frac{1}{2G}\mathbf{\Lambda}_s. \qquad (13.100)$$

Comparison of expressions (13.99) and (13.100) gives the interrelations

$$G = \frac{E}{2(1+v)}, \qquad (13.101)$$

$$K = \frac{E}{d[1 + v(1-d)]}. \qquad (13.102)$$

Interrelation (13.101), unlike (13.102), is independent of the space dimension. Combination of these two equations yields the useful interrelations

$$\frac{d^2}{E} = \frac{1}{K} + \frac{d(d-1)}{2G}, \qquad (13.103)$$

$$v = \frac{dK - 2G}{d(d-1)K + 2G}. \qquad (13.104)$$

Using expression (13.104) and the positivity of K and G, it can be shown that Poisson's ratio v is bounded according to

$$-1 \leq v \leq \frac{1}{(d-1)}. \qquad (13.105)$$

The upper limit of $v = 1/(d-1)$ is obtained from (13.104) by taking the limit that $K/G \to \infty$, i.e., the *incompressible limit*. In three dimensions, when $v \approx 1/2$, as in rubbery solids and liquids, the bulk modulus greatly exceeds the shear modulus. The lower limit of $v = -1$ is found by taking the limit $G/K \to \infty$. For materials with $v \approx -1$, the shear modulus far exceeds the bulk modulus. Elastically isotropic materials having a negative Poisson's ratio, called *auxetic* materials, are extremely rare in nature. However, as discussed in Section 13.3.4, composite materials with negative Poisson's ratio have been devised and fabricated.

Note that one must specify either *plane-strain* or *plane-stress* elasticity when it is desired to connect the moduli for isotropic two-dimensional (planar) elasticity to the

moduli for isotropic three-dimensional elasticity. Plane-strain elasticity is physically relevant in considering a fiber-reinforced material. On the other hand, plane-stress elasticity is physically relevant in considering two-phase composites in the form of thin sheets. The planar shear modulus G (either in plane-strain or plane-stress elasticity) is equal to the three-dimensional shear modulus G. However, the bulk-moduli relations are not as simple. We will follow the convention of denoting the *planar bulk modulus* by k and the three-dimensional bulk modulus by K. The plane-strain bulk modulus k is related to K by the expression

$$k = K + G/3. \tag{13.106}$$

By contrast, the plane-stress bulk modulus k obeys the relation

$$k = \frac{9KG}{3K + 4G}. \tag{13.107}$$

These and other interrelations among the planar and three-dimensional moduli are derived in Appendix B.

13.3.3   Homogenization of Random Problem in $\mathfrak{R}^d$

The homogenization of the elastic problem for periodic media has been given by Sanchez-Palencia (1980). Since the derivation of the homogenized results for random elastic media follows closely the one for periodic elastic media, which in turn is completely analogous to the derivation that we gave previously for the conductivity problem in Section 13.2, we will only sketch the procedure here.

   We recall that each realization ω of the random medium occupies the space $\mathcal{V} \in \mathfrak{R}^d$, which is partitioned into two random sets or phases, as described in the beginning of this chapter (see Figure 13.2). The stiffness tensor is a rapidly oscillating random function of position, which we write as $\boldsymbol{C}^\epsilon(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{y}; \omega)$, where $\boldsymbol{y} = \boldsymbol{x}/\epsilon$ is the fast variable associated with the fineness of the microstructure. As before, it is a *statistically homogeneous function* that is *positive definite* and *bounded*. The displacement $\boldsymbol{u}^\epsilon(\boldsymbol{x}) = \boldsymbol{u}(\boldsymbol{x}, \boldsymbol{y}; \omega)$ satisfies the equilibrium equation for each realization of the ensemble, i.e.,

$$-\frac{\partial}{\partial x_j}\left[C^\epsilon_{ijkl}(\boldsymbol{x})\varepsilon^\epsilon_{kl}(\boldsymbol{x})\right] = f_i(\boldsymbol{x}) \qquad \text{in } \mathcal{V}, \tag{13.108}$$

where $\varepsilon^\epsilon(\boldsymbol{x}) = \varepsilon(\boldsymbol{x}, \boldsymbol{y})$ is the symmetrized gradient of $\boldsymbol{u}^\epsilon$, which we assume is specified on the boundary of $\mathcal{V}$, and $\boldsymbol{f}(\boldsymbol{x})$ is a body force per unit volume.

   When the medium is statistically homogeneous and ergodic, there exists an effective stiffness tensor $(C_e)_{ijkl}$, independent of the boundary conditions in the infinite-volume limit such that if $u^{(0)}_i(\boldsymbol{x})$ is the solution of the *deterministic* equilibrium elasticity equation

$$-(C_e)_{ijkl}\frac{\partial}{\partial x_j}\varepsilon^{(0)}_{kl}(\boldsymbol{x}) = f_i(\boldsymbol{x}), \tag{13.109}$$

where

$$\varepsilon_{ij}^{(0)} = \frac{1}{2}\left[\frac{\partial u_j^{(0)}}{\partial x_i} + \frac{\partial u_i^{(0)}}{\partial x_j}\right], \tag{13.110}$$

then

$$\int_{\mathcal{V}} \langle |\boldsymbol{u}^\epsilon(\boldsymbol{x}) - \boldsymbol{u}^{(0)}(\boldsymbol{x})|^2 \rangle d\boldsymbol{x} \to 0, \quad \text{as } \epsilon \to 0. \tag{13.111}$$

To prove this statement, one begins by assuming the two-scale expansion

$$u_i^\epsilon(\boldsymbol{x}) = u_i^{(0)}(\boldsymbol{x}) + \epsilon u_i^{(1)}(\boldsymbol{x},\boldsymbol{y};\omega) + \epsilon^2 u_i^{(2)}(\boldsymbol{x},\boldsymbol{y};\omega) + \cdots \tag{13.112}$$

of $u_i^\epsilon(\boldsymbol{x})$ and substitute it into (13.108). Proceeding as in the previous section on the effective conductivity, one can show that the effective stiffness tensor is defined by an averaged Hooke's law

$$\langle \boldsymbol{\tau}(\boldsymbol{x}) \rangle = \boldsymbol{C}_e : \langle \boldsymbol{\varepsilon}(\boldsymbol{x}) \rangle, \tag{13.113}$$

where

$$(C_e)_{ijkl} = \langle C_{ijkl} \rangle + \left\langle C_{ijmn}\frac{1}{2}\left(\frac{\partial \chi_{kmn}}{\partial y_l} + \frac{\partial \chi_{lmn}}{\partial y_k}\right)\right\rangle \tag{13.114}$$

and χ_{kmn} is the third-order tensor that solves

$$-\frac{\partial}{\partial y_i}\left[C_{ijkl}(\boldsymbol{y};\omega)\frac{1}{2}\left(\frac{\partial \chi_{kmn}}{\partial y_l} + \frac{\partial \chi_{lmn}}{\partial y_k}\right)\right] = \frac{\partial}{\partial y_i}C_{ijmn}(\boldsymbol{y};\omega) \quad \text{in } \Re^d. \tag{13.115}$$

The definition (13.113) is consistent with the one given in Table 1.1.

Remarks:
1. As in the conductivity problem, macroscopic variation of the effective stiffness tensor could be allowed for; i.e., $\boldsymbol{C}_e(\boldsymbol{x})$ may be assumed to depend on the position $\boldsymbol{x}$, provided that the length scales associated with such variations of $\mathcal{O}(\Lambda)$ are large enough to assume statistical homogeneity at $\boldsymbol{x}$ (local statistical homogeneity).
2. It is shown in Section 14.2.2 that $\boldsymbol{C}_e$ is symmetric and positive definite if the local conductivity tensor $\boldsymbol{C}$ is symmetric and positive definite.
3. In the case of elasticity, *macroscopically isotropic* composites are those whose effective stiffness tensor is specified by

$$\boldsymbol{C}_e = dK_e\boldsymbol{\Lambda}_h + 2G_e\boldsymbol{\Lambda}_s, \tag{13.116}$$

where $\boldsymbol{\Lambda}_h$ and $\boldsymbol{\Lambda}_s$ are the hydrostatic and shear projection tensors given by (13.96) and (13.97), respectively. Similarly, the effective compliance tensor is given by

$$\boldsymbol{S}_e = \frac{1}{dK_e}\boldsymbol{\Lambda}_h + \frac{1}{2G_e}\boldsymbol{\Lambda}_s. \tag{13.117}$$

4. For composites consisting of *isotropic phases*, the following general statements can be made:

- Statistically isotropic composites are always macroscopically isotropic composites [e.g., statistically isotropic arrays of inclusions in a matrix (see Figure 12.6)].

- However, *statistical anisotropy* (as depicted in Figures 7.1 and 16.3, for example) necessarily implies a *macroscopically anisotropic* composite with an effective tensor C_e. This is in contrast to the conduction problem, where statistical anisotropy does not ensure macroscopic anisotropy.

Macroscopically anisotropic elastic composites are not necessarily *statistically anisotropic* if some of the phases are anisotropic. For instance, systems of statistically isotropic arrays of spherical but anisotropic grains oriented in the same direction in an isotropic matrix are macroscopically anisotropic.

5. The effective relation (13.113) applies also to composites with an arbitrary number of phases that meet the standard two-scale assumption.
6. The effective stiffness tensor C_e of a macroscopically anisotropic composite composed of M isotropic phases is a *homogeneous function of degree one* in its $2M$ scalar phase moduli $K_1, G_1, \ldots, K_M, G_M$. For two isotropic phases, this means that $C_e(K_1, G_1, K_2, G_2)$ obeys the relation

$$C_e(\alpha K_1, \alpha G_1, \alpha K_2, \alpha G_2) = \alpha \, C_e(K_1, G_1, K_2, G_2), \qquad \text{for all } \alpha. \tag{13.118}$$

If we set the constant α equal to $1/K_1$, then we get

$$\frac{C_e(K_1, G_1, K_2, G_2)}{K_1} = C_e(1, G_1/K_1, K_2/K_1, G_2/K_1).$$

Thus, the homogeneity property (13.118) enables us to reduce the independent variables from four to three without any loss of generality. The homogeneity property is trivially proven using the effective relation (13.113) and the observation that $\nabla \cdot \boldsymbol{\tau}' = 0$ when $\boldsymbol{\tau}' = \alpha \boldsymbol{\tau}$ and $\nabla \cdot \boldsymbol{\tau} = 0$.

13.3.4   Heterogeneous Materials

It is shown in Section 14.2.2 that if the local stiffness C is both symmetric and positive definite, then the effective stiffness tensor C_e is also symmetric and positive definite. Thus, all of the statements made above concerning the positivity properties and symmetries of the stiffness tensor of homogeneous materials apply as well to C_e. Therefore, there is no need to repeat this entire description for the effective stiffness tensor C_e. However, for future discussion, we describe briefly the effective moduli for transversely isotropic and for isotropic two-phase materials. In particular, we note that in the transversely isotropic case only three moduli (rather than five as in the homogeneous case) are independent.

Transversely Isotropic Composite

Consider a transversely isotropic composite as schematically indicated in Figure 13.6. Generally, such a fiber-reinforced material has phase boundaries that are cylindrical surfaces of arbitrary shape with generators parallel to one axis. Using the procedure
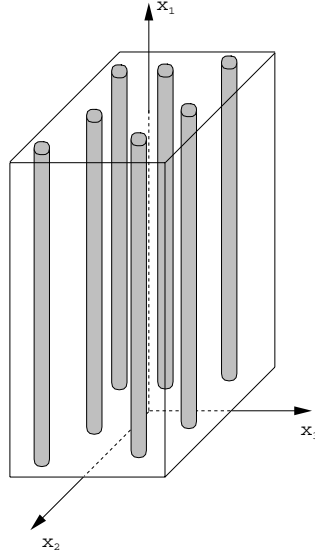
Figure 13.6 A schematic of a fiber-reinforced composite.

given above for homogeneous transversely isotropic materials, it is easily shown that the *average strain–stress* relations are given by

$$\langle \epsilon_{11} \rangle = \frac{1}{E_e^L} \langle \tau_{11} \rangle - \frac{v_e^L}{E_e^L} \langle \tau_{22} \rangle - \frac{v_e^L}{E_e^L} \langle \tau_{33} \rangle, \tag{13.119}$$

$$\langle \epsilon_{22} \rangle = -\frac{v_e^L}{E_e^L} \langle \tau_{11} \rangle + \frac{1}{E_e^T} \langle \tau_{22} \rangle - \frac{v_e^T}{E_e^T} \langle \tau_{33} \rangle, \tag{13.120}$$

$$\langle \epsilon_{33} \rangle = -\frac{v_e^L}{E_e^L} \langle \tau_{11} \rangle - \frac{v_e^T}{E_e^T} \langle \tau_{22} \rangle + \frac{1}{E_e^T} \langle \tau_{33} \rangle, \tag{13.121}$$

$$\langle \epsilon_{12} \rangle = \frac{1}{2G_e^L} \langle \tau_{12} \rangle \, , \ \langle \epsilon_{13} \rangle = \frac{1}{2G_e^L} \langle \tau_{13} \rangle \, , \ \langle \epsilon_{23} \rangle = \frac{1}{2G_e^T} \langle \tau_{23} \rangle, \tag{13.122}$$

where E_e^T, G_e^T, and v_e^T are the effective transverse Young modulus, shear modulus, and Poisson ratio, respectively, and E_e^L, G_e^L, and v_e^L are the effective longitudinal Young modulus, shear modulus, and Poisson ratio, respectively.

There are only five independent effective constants, and thus there are interrelations among the effective moduli. For example, two of them are

$$G_e^T = \frac{E_e^T}{2(1 + v_e^T)}, \tag{13.123}$$

$$\frac{4}{E_e^T} = \frac{1}{k_e^T} + \frac{1}{G_e^T} + \frac{4(v_e^L)^2}{E_e^L}, \tag{13.124}$$

where k_e^T is the transverse bulk modulus *without axial extension* (i.e., $\langle \epsilon_{11} \rangle = 0$). Combining these two relations and taking appropriate limits [as in (13.84)] shows that the effective transverse Poisson ratio lies in the range $-1 \leq v_e^T \leq 1$. A transversely isotropic porous material with negative Poisson's ratios in certain directions was designed using a topology optimization technique and subsequently fabricated using stereolithography (Sigmund, Torquato and Aksay 1998).

Hill (1964) has shown that for the special case of transversely isotropic composites possessing two phases, there are actually only three independent effective properties. For example, if we are given the transverse properties G_e^T, k_e^T and axial property G_e^L, then we can obtain E_e^L and v_e^L through the following relations, which involve only the effective property k_e^T:

$$E_e^L = \langle E \rangle + \frac{4(v_2 - v_1)^2}{\left(\dfrac{1}{k_2^T} - \dfrac{1}{k_1^T} \right)^2} \left(\left\langle \frac{1}{k^T} \right\rangle - \frac{1}{k_e^T} \right), \tag{13.125}$$

$$v_e^L = \langle v \rangle - \frac{(v_2 - v_1)}{\left(\dfrac{1}{k_2^T} - \dfrac{1}{k_1^T} \right)} \left(\left\langle \frac{1}{k^T} \right\rangle - \frac{1}{k_e^T} \right), \tag{13.126}$$

where $k_i^T = K_i + G_i/3$ is the transverse bulk modulus for phase i.

Isotropic Composite

From the discussion above for homogeneous isotropic materials, it is clear that the averaged stress–strain and strain–stress relations in any space dimension d are given respectively by

$$\langle \tau_{ij} \rangle = K_e \langle \epsilon_{kk} \rangle \delta_{ij} + 2G_e \left[\langle \epsilon_{ij} \rangle - \langle \epsilon_{kk} \rangle \frac{\delta_{ij}}{d} \right], \qquad i,j = 1, \ldots, d, \tag{13.127}$$

$$\langle \varepsilon_{ij} \rangle = -\frac{v_e}{E_e} \langle \tau_{kk} \rangle \delta_{ij} + \frac{1 + v_e}{E_e} \langle \tau_{ij} \rangle, \qquad i,j = 1, \ldots, d, \tag{13.128}$$

where

$$K_e = \lambda_e + \frac{2}{d} G_e \tag{13.129}$$

is the effective bulk modulus, λ_e is the effective Lamé constant, G_e is the effective shear modulus, E_e is the effective Young modulus, and v_e is the effective Poisson ratio. Of course, these effective Hooke's laws could also have been obtained using (13.113), (13.116), and (13.117). Interrelations between the effective moduli can be obtained in exactly the same way as for a homogeneous isotropic material. For example, we have

$$G_e = \frac{E_e}{2(1 + v_e)}, \quad K_e = \frac{E_e}{d[1 + v_e(1 - d)]}, \quad \frac{d^2}{E_e} = \frac{1}{K_e} + \frac{d(d - 1)}{2G_e}. \tag{13.130}$$

The analogue of (13.104) for an isotropic composite is the expression

$$v_e = \frac{dK_e - 2G_e}{d(d-1)K_e + 2G_e} \tag{13.131}$$

for the effective Poisson ratio. Using similar arguments as before, we see that v_e is bounded by

$$-1 \leq v_e \leq \frac{1}{(d-1)}. \tag{13.132}$$

Elastically isotropic auxetic composites (i.e., $v_e < 0$) have been devised and/or fabricated. Hierarchical laminates (Chapter 16) can exhibit extremal Poisson's ratio approaching -1 (Milton 1992). Auxetic foams with *reentrant* (i.e., nonconvex) cell structures have been fabricated (Lakes 1987). In two dimensions, analogous auxetic cellular materials have been designed and fabricated (Sigmund 1994, Larsen, Sigmund and Bouwstra 1997, Xu, Arias, Brittain, Zhao, Gryzbowski, Torquato and Whitesides 1999). One may also achieve a Poisson ratio of -1 by a two-dimensional chiral honeycomb structure (Prall and Lakes 1997).

13.3.5   Relationship Between Elasticity and Viscous Fluid Theory

There is a well-known connection between linear elasticity and slow viscous flow of a fluid that is worth noting here. Consider time-dependent phenomena and let us write the *equations of motion* for a homogeneous material in terms of the displacement $\boldsymbol{u}$, i.e.,

$$(\lambda + G)\, \nabla(\nabla \cdot \boldsymbol{u}) + G\, \Delta \boldsymbol{u} + \boldsymbol{f} = \rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2},$$

where ρ is the mass density and t is time. Now, in the case of an *incompressible* material, we have the solenoidal condition

$$\nabla \cdot \boldsymbol{u} = 0,$$

but incompressibility also means that $K \rightarrow \infty$ or $\lambda \rightarrow \infty$. Thus, the first term in the momentum equation is indeterminate and can be written in terms of the reactive hydrostatic pressure p, giving

$$-\nabla p + G\, \Delta \boldsymbol{u} + \boldsymbol{f} = \rho\, \frac{\partial^2 \boldsymbol{u}}{\partial t^2}. \tag{13.133}$$

Let us now compare the expression above to the Navier–Stokes equations of motion for an *incompressible Newtonian viscous fluid*, i.e.,

$$-\nabla p + \mu\, \Delta \boldsymbol{v} + \boldsymbol{f} = \rho \left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} \right),$$

where $\boldsymbol{v}$ is the velocity vector, $\boldsymbol{f}$ is a body force per unit volume, p is the pressure, and μ is the dynamic viscosity. Conservation of mass for an incompressible fluid is expressed by the condition
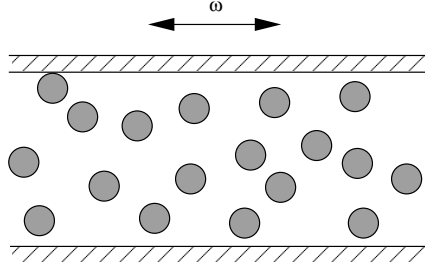
$$\nabla \cdot \boldsymbol{v} = 0.$$

Figure 13.7   Suspension of rigid particles in an incompressible fluid between a plate that harmonically oscillates with frequency ω and a fixed plate. In the limit $\omega \to \infty$, the determination of the effective viscosity μ_e becomes equivalent to finding the steady-state effective shear modulus G_e of rigid particles (with the same configuration) in an incompressible matrix.

For slow viscous flow (Reynolds number going to zero), the nonlinear inertial term $v \cdot \nabla v$ can be shown to be very small compared to the rest of the terms, and thus we obtain the *creeping flow* equations

$$-\nabla p + \mu \, \Delta v + f = \rho \frac{\partial v}{\partial t}. \tag{13.134}$$

Thus, under steady-state conditions, the creeping flow equations (13.134) are identical to the governing elasticity equations (13.133) for incompressible materials when *u* and G are identified with v and μ, respectively. The time-dependent equations (13.134) will be employed in Section 13.8.

13.3.6   Viscosity of a Suspension

Under certain conditions, obtaining the effective viscosity μ_e of a suspension of perfectly rigid particles ($\mu_2 \to \infty$) in an incompressible fluid with viscosity μ_1 (under creeping flow conditions) is equivalent to finding the *steady-state* effective shear modulus G_e of a composite composed of the same perfectly rigid particles in an incompressible matrix with shear modulus G_1, i.e.,

$$\frac{\mu_e}{\mu_1} = \frac{G_e}{G_1}. \tag{13.135}$$

Relation (13.135) is exact when hydrodynamic interactions between the particles can be neglected (i.e., at infinitely dilute conditions $\phi_2 \to 0$), regardless of the configuration of the particles. At nondilute conditions, (13.135) is also exact, provided that the configurations of the particles in the flow and elasticity problems are identical. This situation is realized for arbitrary particle concentrations when the fluid is subjected to an applied oscillating shear rate with frequency ω in the infinite-frequency limit ($\omega \to \infty$), as depicted in Figure 13.7. However, for finite frequencies in the flow problem at nondilute conditions, the configuration of the particles changes with time and

is not known in advance (Russel et al. 1989), and thus relation (13.135) generally does not hold.

13.3.7   Viscoelasticity

Many composite materials, particularly those possessing a polymeric phase, will exhibit a time and rate dependence that is not captured by elasticity theory. In these materials deformations grow (creep), stresses relax, and mechanical vibrations are damped. These effects are magnified at elevated temperatures. Such materials are said to be *viscoelastic*, since they display aspects of both viscous and elastic types of behavior. Under quasi-static conditions (when inertial effects are negligibly small), there is a well-known exact connection between the elastic and viscoelastic problems called the *elastic–viscoelastic correspondence principle* (Hashin 1965a, Christensen 1979). If the time-domain viscoelastic equations are Laplace transformed, then this principle states that the static elastic problem can be converted to the transformed solutions of the viscoelastic problem by simply replacing the static stiffness tensor C_e with $s\hat{C}_e(s)$, where s is the transform variable and $\hat{C}_e(s)$ is the Laplace transform of the time-dependent stiffness $C(t)$. The determination of the quasi-static tensor $C(t)$ is found via a transform inversion.

Under steady-state harmonic conditions at sufficiently low values of the frequency ω, the correspondence principle is even simpler. The complex viscoelastic stiffness $C^*(\omega)$ can be found from formulas for the static effective stiffness C_e by replacing the real elastic moduli with their complex counterparts. For composite materials, the quasi-static condition is satisfied if the heterogeneity length scale is much smaller than the wavelength. Viscoelasticity will not be covered in any detail in this book. The reader is referred to Hashin (1965a) and Christensen (1979) and references therein for pertinent literature on this subject.

13.4   Steady-State Trapping Problem

Consider the problem of diffusion and reaction among *partially absorbing* "traps" in each realization ω of the random medium defined in Section 13.1. Let $\mathcal{V}_1(\omega)$ be the region in which diffusion occurs (i.e., trap-free, or pore, region) and let $\mathcal{V}_2(\omega)$ be the trap region. The concentration field of the reactants $c(x, y; \omega)$ at position x exterior to the traps at time t is generally governed by the mass conservation equation

$$\frac{\partial c}{\partial t} = \mathcal{D}\Delta c - \kappa_B c + G \qquad \text{in } \mathcal{V}_1(\omega) \tag{13.136}$$

with the boundary condition at the pore–trap interface given by

$$\mathcal{D}\frac{\partial c}{\partial n} + \kappa c = 0 \qquad \text{on } \partial\mathcal{V}(\omega) \tag{13.137}$$
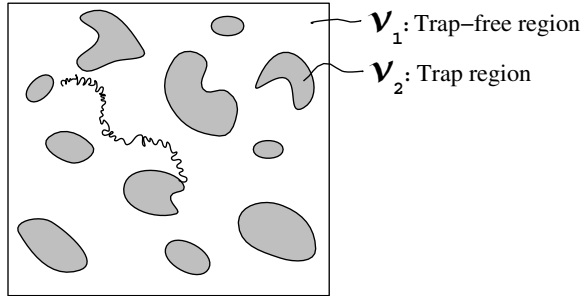
Figure 13.8 A schematic of the "trapping" problem with a static trap phase. Diffusion occurs in the trap-free (or pore) region. A diffusing particle (indicated by the erratic trajectory) is absorbed at the pore–trap interface with a probability related to the surface rate constant κ.

and some specified initial condition and boundary conditions. Here $\mathcal{D}$ is the diffusion coefficient of the reactant, κ_B is a positive bulk rate constant, κ is a positive surface rate constant, G is a generation rate per unit trap-free volume, and $\boldsymbol{n}$ is the unit outward normal from the pore space. Without loss of generality, one can set the bulk rate constant κ_B equal to zero: The solution $c(\boldsymbol{x}, t)$ of (13.136) with $\kappa_B \neq 0$ multiplied by $\exp(\kappa_B t)$ gives the corresponding solution with $\kappa_B = 0$. However, for the steady-state problems mentioned below, the solution $c(\boldsymbol{x}; \omega)$ for $\kappa_B = 0$ is not simply related to the solution $c(\boldsymbol{x}; \omega)$ for $\kappa_B \neq 0$ (Talbot and Willis 1984).

It is useful to introduce the dimensionless surface rate constant

$$\kappa^* = \frac{\kappa \ell}{\mathcal{D}}, \tag{13.138}$$

where ℓ is a characteristic pore length scale, and distinguish between two extreme regimes:

$$\begin{aligned}
\kappa^* &\gg 1 \quad \text{(diffusion-controlled)}, \\
\kappa^* &\ll 1 \quad \text{(reaction-controlled)}.
\end{aligned} \tag{13.139}$$

In the *diffusion-controlled* regime, the diffusing species takes a long time to diffuse to the pore–trap interface relative to the characteristic time associated with the surface reaction; i.e., the process is governed by diffusion. For infinite surface reaction ($\kappa = \infty$), the traps are perfect absorbers, and thus the interface condition is of the *Dirichlet* kind, with $c = 0$. On the other hand, in the *reaction-controlled* regime, the characteristic time associated with surface reaction is large compared with the diffusion time to the pore–trap interface. For vanishing surface reaction ($\kappa = 0$), the traps are perfect reflectors, and hence the interface condition is of the *Neumann* kind, with $\partial c / \partial n = 0$.

We will study relation (13.136) with condition (13.137) for two different situations: (i) the *steady-state* solution with $\kappa_B = 0$ and (ii) the *time-dependent* solution with $\kappa_B = G = 0$. The quantities of central interest for these problems are respectively (i) the *mean survival time* τ of a Brownian particle and (ii) the *relaxation times* T_n, which are inversely proportional to the eigenvalues. The times τ and T_1 are intimately linked

to characteristic length scales of the pore region. Whereas the mean survival time τ is determined by the "average pore size," the *principal* (largest) relaxation time T_1 is governed by diffusion occurring in the largest cavities (pores) in the system. The steady-state trapping will be discussed in the present section. The time-dependent problem will be considered in Section 13.7.

13.4.1   Local Relations

Consider the steady-state problem of diffusion and reaction among perfectly absorbing traps ($\kappa = \infty$). The rate of production of the reactants per unit volume G is exactly compensated by the rate of removal by the traps.

Local Differential Equation

The conservation of mass equation (13.136) under steady-state conditions and without bulk reaction reduces to the following Poisson equation for the concentration field $c(x; \omega)$:

$$\mathcal{D}\Delta c = -G \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.140}$$

$$c = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.141}$$

Henceforth, we will assume a zero-flux condition at the boundary of $\mathcal{V}$ (macroscopic sample surface). However, as we have emphasized throughout this chapter, the effective property (trapping constant in this case) is independent of the macroscopic boundary conditions for ergodic media.

13.4.2   Homogenization of Random Problem in $\mathfrak{R}^d$

What is the appropriate *macroscopic* constitutive relation for the steady-state trapping problem? In the chemical physics literature (Prager 1963a, Calef and Deutch 1983), it is assumed that the trapping constant γ (a quantity that will be shown to be inversely proportional to τ) obeys the first-order rate equation

$$G = \gamma\mathcal{D}C, \tag{13.142}$$

where C represents an average concentration field. To derive this constitutive relation rigorously from homogenization theory, we follow the treatment of Rubinstein and Torquato (1988) for the case of perfectly absorbing traps ($\kappa = \infty$).

In general, it is assumed that there exists a small parameter $\epsilon = \ell/L$ associated with rapid fluctuations in the structure of $\mathcal{V}_1(\omega)$ and that the concentration field c depends on two scales: a slow scale x and a fast scale $y = x/\epsilon$. Thus, $c^\epsilon(x) = c(x, y; \omega)$ satisfies

$$\mathcal{D}\Delta c^\epsilon(x) = -G(x) \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.143}$$

$$c^\epsilon(x) = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.144}$$

In order to derive the macroscopic behavior, we assume that c^ϵ admits a two-scale expansion of the form

$$c^\epsilon(\boldsymbol{x}) = \epsilon^2 c_0(\boldsymbol{x}, \boldsymbol{y}; \omega) + \epsilon^3 c_1(\boldsymbol{x}, \boldsymbol{y}; \omega) + \cdots, \tag{13.145}$$

in contrast to the previous two problems [cf. (13.45) and (13.112)]. Note that the first nontrivial term in this expansion for c^ϵ is $\mathcal{O}(\epsilon^2)$, in contrast to the expansion (13.45) for T^ϵ. Physically, this expansion arises because an $\mathcal{O}(1)$ production rate gives a concentration of $\mathcal{O}(\epsilon^2)$. Substitution of this expansion into relation (13.143) and use of the identities

$$\nabla = \nabla_x + \frac{1}{\epsilon}\nabla_y, \qquad \Delta \equiv \nabla^2 = \Delta_x + \frac{2}{\epsilon}\nabla_x \cdot \nabla_y + \frac{1}{\epsilon^2}\Delta_y \tag{13.146}$$

yields

$$\mathcal{D}\left(\frac{1}{\epsilon^2}\Delta_y + \frac{2}{\epsilon}\nabla_x \cdot \nabla_y + \Delta_x\right)\left(\epsilon^2 c_0 + \epsilon^3 c_1 + \cdots\right) = -G(\boldsymbol{x}).$$

Therefore, the leading-order equation is given by

$$\mathcal{D}\Delta_y c_0(\boldsymbol{x}, \boldsymbol{y}; \omega) = -G(\boldsymbol{x}) \qquad \text{in } \mathcal{V}_1(\omega),$$
$$c_0(\boldsymbol{x}, \boldsymbol{y}; \omega) = 0 \qquad \text{on } \partial\mathcal{V}(\omega).$$

Hence, we can write

$$c_0 = \mathcal{D}^{-1}G(\boldsymbol{x})u(\boldsymbol{y}; \omega), \tag{13.147}$$

where the scaled auxiliary concentration field u solves

$$\Delta_y\, u(\boldsymbol{y}; \omega) = -1 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.148}$$
$$u(\boldsymbol{y}; \omega) = 0 \qquad \text{on } \partial\mathcal{V}(\omega), \tag{13.149}$$

and we extend u in the trap region $\mathcal{V}_2(\omega)$ to be zero. Assuming that the medium is locally (i.e., on the fast scale) statistically homogeneous and ergodic, the ensemble average of any function $g(\boldsymbol{x}, \boldsymbol{y}; \omega)$ is simply a function of $\boldsymbol{x}$ only. Averaging (13.147) gives the constitutive relation

$$G(\boldsymbol{x}) = \gamma\mathcal{D}C(\boldsymbol{x}), \tag{13.150}$$

where

$$C(\boldsymbol{x}) = \langle c_0(\boldsymbol{x}, \boldsymbol{y}; \omega)\rangle$$

and the constant γ, called the *trapping constant*, is given by

$$\gamma^{-1} = \langle u(\boldsymbol{y}; \omega)\rangle = \langle u\mathcal{I}^{(1)}\rangle. \tag{13.151}$$

We see that relation (13.150) agrees with (13.142) but additionally allows for slow spatial variations in C and G.

Remarks:
1. The trapping problem is fundamentally different than the previous two problems. Here there is no local constitutive relation. Moreover, the trapping constant γ has
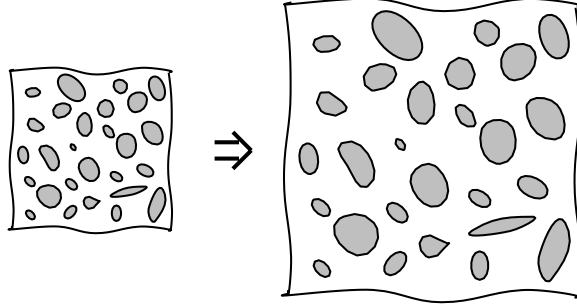
Figure 13.9 A schematic illustrating the scale-dependence of both the trapping constant γ (for perfectly absorbing traps) and fluid permeability tensor k. If the linear dimensions of the porous medium are doubled, then the new trapping constant is four times smaller than the original one, whereas the components of the new fluid permeability tensor are four times larger than the original components.

dimensions (length)$^{-2}$ and therefore, unlike the effective conductivity or elastic moduli, is a scale-dependent property. Thus, if we apply an affine transformation to the system in each of the space coordinates (i.e., rescale each coordinate by some constant factor α), then the trapping constant γ' of the new system is related to the trapping constant γ of the original system via $\gamma' = \gamma/\alpha^2$ (see Figure 13.9). As discussed in the next section, the fluid permeability tensor k is also a scale-dependent property.

2. What is the physical interpretation of the trapping constant γ? Dimensional analysis of (13.150) reveals that γ has dimensions of (length)$^{-2}$, since $\mathcal{D}$ has dimensions of (length)^2 per unit time, C has dimensions of inverse volume, and G has dimensions of inverse volume per unit time. Consider a constant production rate G. Now let the total number of diffusing (Brownian) particles created outside of traps per unit time be N and the total number of particles exterior to traps at a given time be N_0. Then the *average trapping rate* k_R (per particle) is given by

$$k_R = \frac{N}{N_0}.$$

The inverse of this quantity, called the *mean survival time* τ of a Brownian particle, is thus given by

$$\tau = k_R^{-1} = \frac{N_0}{N}.$$

It is clear that

$$N = GV_1, \qquad N_0 = CV,$$

where V_1 is the volume of phase 1 and V is the total volume. Use of the relations immediately above and definition (13.151) allows us to write

$$\tau = \frac{1}{\gamma \phi_1 \mathcal{D}} = \frac{\langle u \rangle}{\phi_1 \mathcal{D}}. \tag{13.152}$$

Thus, the trapping constant γ is proportional to the trapping rate k_R or inversely proportional to the mean survival time τ. Roughly speaking, the quantity γ^{-1} provides a measure of the *average pore size*. In subsequent discussions we will refer to both the trapping constant γ and the mean survival time τ. We note that substitution of (13.152) into (13.150) yields the corresponding constitutive relation defining τ, i.e.,

$$C(x) = \tau \phi_1 G(x). \tag{13.153}$$

We see that this definition is consistent with the one given in Table 1.1.

3. Since γ does not vanish when the trap-free region becomes disconnected, the trapping constant does not exhibit *percolation* or *critical* behavior. This is in contrast to the effective conductivity, effective stiffness, and fluid permeability, which are affected by phase connectedness and hence do exhibit percolation behavior.

4. Unlike the effective conductivity, effective stiffness, or fluid permeability, the trapping constant γ remains a scalar quantity even if the microstructure is statistically anisotropic [e.g., arrays of oriented cylinders or ellipsoids (see Figure 7.1)].

5. It is important to note that in the case of finite surface reaction ($\kappa < \infty$), i.e., when u solves

$$\Delta_y \, u(y; \omega) = -1 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.154}$$

$$\mathcal{D}\frac{\partial u}{\partial n} + \kappa u = 0 \qquad \text{on } \partial \mathcal{V}(\omega), \tag{13.155}$$

the averaged relation (13.151) still defines the trapping constant.

13.5   Steady-State Fluid Permeability Problem

It is well established that the slow flow of an incompressible viscous fluid through porous media is often described by Darcy's law (Scheidegger 1974):

$$U = -\frac{k}{\mu}\nabla p_0, \tag{13.156}$$

where U is the average fluid velocity, ∇p_0 is the applied pressure gradient, μ is the *dynamic viscosity*, and k is the *fluid permeability*. Figure 13.10 depicts a porous medium and the relevant flow parameters. The permeability k has dimensions of (length)^2 and, roughly speaking, may be regarded as an *effective pore channel area of the dynamically connected part of the pore space*.

We refer to the portion of the *connected* pore space that carries an appreciable part of the flow (say, above some designated flow rate) as the "dynamically connected" part of the pore space. However, there will be regions of connected pore space that carry no appreciable flow, and such regions contribute negligibly to the fluid permeability.
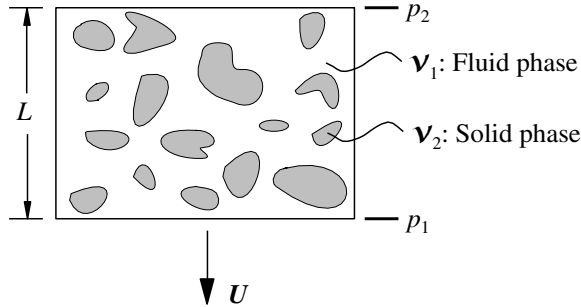
Figure 13.10 A schematic of a porous medium indicating the applied pressure drop $(p_2 - p_1)/L$ and average velocity U that determine the permeability k in Darcy's law.
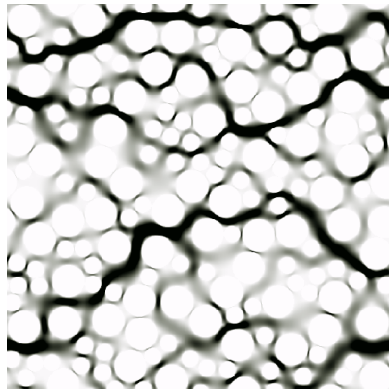

Figure 13.11 Gray-scale image of fluid speeds in a Stokes-flow simulation of a two-dimensional flow past a bed of two different-sized disks as computed by N. Martys at the National Institute of Standards and Technology. Black and white pore regions indicate highest fluid speeds and no flow, respectively. Similar images can be found in Martys and Garboczi (1992).

Therefore, permeability estimates for general porous media based on purely simple pore statistics, such as porosity and specific surface, are inherently fundamentally unsound. Figure 13.11 beautifully illustrates the idea that only a subset of the pore space contributes to the fluid permeability.

13.5.1 Local Relations

For each realization ω of the random porous medium, let $\mathcal{V}_1(\omega)$ be the region through which the fluid flows (i.e., pore, or void, region) and let $\mathcal{V}_2(\omega)$ be the solid region.

Local Differential Equations

The fluid motion satisfies the Stokes equations

$$\mu\Delta v = \nabla p \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.157}$$

$$\nabla \cdot v = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.158}$$

$$v = 0 \qquad \text{on } \partial\mathcal{V}(\omega), \tag{13.159}$$

where v and p are the local velocity and pressure fields, respectively. The first relation is the steady-state momentum equation in the limit of vanishing Reynolds number, the second relation states that the fluid is incompressible, and the last relation is the no-slip condition on the pore–solid interface. Henceforth, we will assume a zero-traction condition on the boundary of $\mathcal{V}$ (macroscopic sample boundary), but since we are interested ultimately in ergodic media, the permeability will not depend on the details of the boundary conditions.

13.5.2   Homogenization of Random Problem in $\mathfrak{R}^d$

Darcy's law has been derived using the method of homogenization by Sanchez-Palencia (1980) for periodic media and by Rubinstein and Torquato (1989) for random media. Let us consider the *random* setting in which the medium is taken generally to be *macro-scopically anisotropic*. The porous medium, which occuipes space $\mathcal{V}(\omega) \in \mathfrak{R}^d$, is assumed to have a microscopic length scale ℓ (e.g., the scale over which $\mathcal{I}^{(1)}$ varies) that is small compared to a typical macroscopic length scale L. Again, there is a small parameter $\epsilon = \ell/L$, and we assume that the velocity v and pressure p depend on two scales: a slow scale x and a fast scale $y = x/\epsilon$. Therefore, $v^\epsilon(x) = v(x, y; \omega)$ and $p^\epsilon(x) = p(x, y; \omega)$ satisfy

$$\mu\Delta v^\epsilon(x) = \nabla p^\epsilon(x) \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.160}$$

$$\nabla \cdot v^\epsilon(x) = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.161}$$

$$v^\epsilon(x) = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.162}$$

To derive the macroscopic equations, we assume a two-scale expansion

$$v^\epsilon(x) = \epsilon^2 v_0(x, y; \omega) + \epsilon^3 v_1(x, y; \omega) + \cdots,$$

$$p^\epsilon(x) = p_0(x) + \epsilon\, p_1(x, y; \omega) + \cdots.$$

Note that the first nontrivial term in the expansion for the velocity is $\mathcal{O}(\epsilon^2)$, in contrast to the expansion for the pressure. Physically, this expansion arises because an $\mathcal{O}(1)$ pressure gives a velocity of $\mathcal{O}(\epsilon^2)$. Substitution of these relations into the Stokes equations (13.160)–(13.162) gives the leading-order equations as

$$\mu\Delta_y v_0(x, y; \omega) = \nabla_y\, p_1(x, y; \omega) + \nabla_x\, p_0(x) \quad \text{in } \mathcal{V}_1(\omega), \tag{13.163}$$

$$\nabla_y \cdot v_0(x, y; \omega) = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.164}$$

$$\nabla_x \cdot v_0(x, y; \omega) + \nabla_y \cdot v_1(x, y; \omega) = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.165}$$

$$v_0(x, y; \omega) = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.166}$$

Here we have used the identities of (13.146). We assume that the medium is locally (i.e., on the fast scale) statistically homogeneous and ergodic, and hence ensemble averaging (13.165) yields

$$\nabla_x \cdot \boldsymbol{U}(\boldsymbol{x}) + \langle \nabla_y \cdot \boldsymbol{v}_1(\boldsymbol{x},\boldsymbol{y};\omega) \rangle = 0, \tag{13.167}$$

where

$$\boldsymbol{U}(\boldsymbol{x}) = \langle \boldsymbol{v}_0(\boldsymbol{x},\boldsymbol{y};\omega) \rangle. \tag{13.168}$$

By integrating by parts and using Gauss's divergence theorem (see Chapter 14 for details), it can be shown that

$$\langle \nabla_y \cdot \boldsymbol{v}_1(\boldsymbol{x},\boldsymbol{y};\omega) \rangle = 0, \tag{13.169}$$

and hence

$$\nabla_x \cdot \boldsymbol{U}(\boldsymbol{x}) = 0. \tag{13.170}$$

Relation (13.170) is just the *macroscopic* incompressibility condition.

In order to analyze (13.163) and (13.164), we introduce the following statistically homogeneous random functions: a second-order tensor "velocity" field $\boldsymbol{w}(\boldsymbol{y};\omega)$ and a vector "pressure" field $\boldsymbol{\pi}(\boldsymbol{y};\omega)$. These quantities are solutions of

$$\Delta_y \boldsymbol{w} = \nabla_y \boldsymbol{\pi} - \boldsymbol{I} \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.171}$$

$$\nabla_y \cdot \boldsymbol{w} = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.172}$$

$$\boldsymbol{w} = 0 \qquad \text{on } \partial\mathcal{V}(\omega), \tag{13.173}$$

where $\boldsymbol{I}$ is the second-order unit tensor. In these equations the scaled tensor velocity field w_{ij} is the jth component of the velocity due to a unit pressure gradient in the ith direction, and π_j is the jth component of the associated scaled pressure. Note that w_{ij} is generally not symmetric. We extend $\boldsymbol{w}$ and $\boldsymbol{\pi}$ in the solid region $\mathcal{V}_2$ to be zero. It is easily seen that v_0 and p_1 can be written as

$$\boldsymbol{v}_0(\boldsymbol{x},\boldsymbol{y};\omega) = -\frac{1}{\mu} \nabla p_0(\boldsymbol{x}) \cdot \boldsymbol{w}(\boldsymbol{y};\omega), \tag{13.174}$$

$$p_1(\boldsymbol{x},\boldsymbol{y};\omega) = \nabla p_0(\boldsymbol{x}) \cdot \boldsymbol{\pi}(\boldsymbol{y};\omega). \tag{13.175}$$

Averaging (13.174) gives

$$\boldsymbol{U}(\boldsymbol{x}) = -\frac{1}{\mu} \langle \boldsymbol{w}(\boldsymbol{y};\omega) \rangle \cdot \nabla p_0(\boldsymbol{x}).$$

The second-order permeability tensor $\boldsymbol{k}$ is then defined by

$$\boldsymbol{k} = \langle \boldsymbol{w}(\boldsymbol{y};\omega) \rangle. \tag{13.176}$$

In summary, the macroscopic equations that govern the slow viscous flow through an anisotropic porous medium are given by

$$\boldsymbol{U}(\boldsymbol{x}) = -\frac{\boldsymbol{k}}{\mu} \cdot \nabla p_0(\boldsymbol{x}), \tag{13.177}$$

$$\nabla \cdot \boldsymbol{U}(\boldsymbol{x}) = 0, \tag{13.178}$$

where $\boldsymbol{k}$ is given by (13.176). Observe that this definition is consistent with the one given in Table 1.1.

Remarks:

1. The fluid permeability shares some similarities with the trapping constant (or mean survival time) but is fundamentally different from either the effective conductivity or effective elastic moduli. As in the trapping problem, there is no local constitutive relation in the flow problem. Furthermore, both the fluid permeability and trapping constant are scale-dependent properties, in contrast to both the effective conductivity and elastic moduli, which are scale-invariant properties. Thus, if we apply an affine transformation to the system in each of the space coordinates, i.e., rescale each coordinate by some constant factor α, then the permeability of the new system, k', is related to that of the original system, k, via $k' = \alpha^2 k$ (see Figure 13.9).
2. The permeability tensor k is given in terms of the random boundary value problem (13.171)–(13.173) and is shown to be symmetric and positive definite in Section 14.4.1.
3. If the medium is macroscopically isotropic, then $k = kI$, where $k = \langle w : I \rangle / d$ is a scalar. In such instances, the auxiliary tensor equations (13.171)–(13.173) become vector equations; i.e., the scalar permeability is redefined as

$$k = \langle w \cdot e \rangle, \tag{13.179}$$

where the scaled *vector* velocity w solves

$$\Delta w = \nabla \pi - e \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.180}$$

$$\nabla \cdot w = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.181}$$

$$w = 0, \qquad \text{on } \partial \mathcal{V}(\omega). \tag{13.182}$$

In these equations, π is the scaled *scalar* pressure field, e is a unit vector, and the subscript y has been dropped.
4. Whereas statistically isotropic porous media are always macroscopically isotropic, statistical anisotropy does not necessarily imply a *macroscopically anisotropic* porous medium with an effective fluid permeability tensor k. For instance, porous media with cubic symmetry are statistically anisotropic but are macroscopically isotropic (e.g., cubic lattices of spheres). Macroscopically anisotropic porous media are necessarily *statistically anisotropic* [e.g., statistically anisotropic beds of oriented cylinders or ellipsoids (see Figure 7.1) or stratified media (see Figure 16.3)].

13.5.3   Relationship to Sedimentation Rate

The problem of the sedimentation of macroscopic particles in a viscous liquid is related to that of flow in a porous medium composed of a fixed bed of particles. In the former, one is interested in finding the *mobility*, which is the constant of proportionality in the relation between the average sedimentation velocity (relative to zero-flux axes) and the force acting on a particle (assuming identical particles); see Table 1.1. One can see that this sedimentation constitutive law bears a strong resemblance to Darcy's law, since the pressure gradient is related to the average force acting on a particle (see Sections

18.4 and 19.4). However, the mobility and permeability are generally not related in a simple manner; the physics of the particle interactions are quite different in the two problems. In the sedimentation problem the particles are free to move, and there is backflow, whereas in the porous-medium problem the particles are fixed, resulting in *screened* interactions. We note that if the relative particle positions are kept fixed during sedimentation, the sedimentation velocity is trivially related to the permeability for the same particle configuration in the infinite-volume limit. This idealized situation was studied for the case of spheres fixed on the sites of cubic lattices (Sangani and Acrivos 1982, Zick and Homsy 1982). The reader is referred to Brady and Durlofsky (1988) and references therein for further discussion on the sedimentation problem.

13.6   Classification of Steady-State Problems

The aforementioned steady-state problems have been designated as falling within classes A, B, C, or D in Section 13.1 and Table 1.1. This classification scheme is somewhat vague, and therefore in this section we make it more mathematically precise. First, we will reserve the symbol α to designate processes that are characterized by a local constitutive relation (e.g., A and B problems) and the symbol β to designate processes that are *not* characterized by a local constitutive relation (e.g., C and D problems).

Our classification scheme is based on the fact that all problems are described by an averaged constitutive relation of a particular tensorial order involving a local generalized flux field that satisfies a conservation equation of a certain tensorial order. In the case of conduction, we see that the averaged constitutive relation (13.46) transforms the vector $\langle E \rangle$ (a first-order tensor) into the vector $\langle J \rangle$ (another first-order tensor). The associated conservation equation for the local flux (13.3) is a scalar equation (a zeroth-order tensor). Thus, the conduction problem and all mathematically equivalent problems are said to fall within class $\alpha(1, 1; 0)$, where the first two arguments indicate a transformation from a first-order tensor to a first-order tensor, and the last argument indicates the order of the conservation equation. In general, class $\alpha(m, n; p)$ describes transformations from an mth-order tensor to an nth-order tensor with a local flux field that satisfies a pth-order tensor conservation equation. The effective property must therefore be a tensor of order $(m + n)$. Thus, classes A and B are more precisely defined according to the following prescription:

$$A \equiv \alpha(1, 1; 0), \tag{13.183}$$
$$B \equiv \alpha(2, 2; 1). \tag{13.184}$$

The second statement follows immediately from the averaged Hooke's law (13.113) and the conservation (equilibrium) equation (13.50). We could make the classification scheme even more elaborate (e.g., one can account for equations governing the generalized intensity field, interface conditions, etc.) but do not do so for the sake of simplicity.

Following the same prescription, we see that classes *C* and *D* are defined as follows:

$$C \equiv \beta(0, 0; 0), \tag{13.185}$$

$$D \equiv \beta(1, 1; 1). \tag{13.186}$$

The first statement follows from the constitutive relation (13.153) and the diffusion equation (13.140). The second statement follows from Darcy's law (13.156) and the momentum relation in the Stokes equations (13.157).

The above classification scheme can be extended to include coupled phenomena, such as thermoelectricity, thermoelasticity, piezoelectricity, and magnetoelasticity.

13.7   Time-Dependent Trapping Problem

The relaxation times associated with the decay of physical quantities such as the concentration field or nuclear magnetization density are related closely to the characteristic length scales of the pore of the fluid region. In what follows we describe the basic equations and note certain connections to the steady-state trapping problem.

13.7.1   Basic Equations

Let $c(\boldsymbol{x}, t)$ denote the physical quantity of interest (e.g., concentration, magnetization density) at local position $\boldsymbol{x}$ and time t, obeying the time-dependent diffusion equation

$$\frac{\partial c}{\partial t} = \mathcal{D}\triangle c + c_o \delta(t) \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.187}$$

$$\mathcal{D}\frac{\partial c}{\partial n} + \kappa c = 0 \qquad \text{on } \partial\mathcal{V}(\omega), \tag{13.188}$$

in a *finite* but *large* pore region $\mathcal{V}_1$. Here c_o is the initial constant concentration field and $\delta(t)$ is the Dirac delta function. In all of the ensuing discussion we will assume a zero-flux condition on the boundary of $\mathcal{V}$.

The solution of (13.187) and (13.188) can be expressed as an expansion in orthonormal functions $\{\psi_n\}$:

$$\frac{c(\boldsymbol{x}, t)}{c_o} = \sum_{n=1}^{\infty} a_n e^{-t/T_n} \psi_n(\boldsymbol{x}), \tag{13.189}$$

where

$$\triangle\psi_n = -\lambda_n \psi_n \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.190}$$

$$\mathcal{D}\frac{\partial\psi_n}{\partial n} + \kappa\psi_n = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.191}$$

The diffusion relaxation times T_n are related to the eigenvalues λ_n by

$$T_n = \frac{1}{\mathcal{D}\lambda_n}. \tag{13.192}$$

At long times, the smallest eigenvalue λ_1, or principal (largest) relaxation time T_1, dominates. The initial condition and the normal mode expansion (13.189) give

$$\sum_{n=1}^{\infty} a_n \psi_n(\boldsymbol{x}) = 1. \tag{13.193}$$

The eigenfunctions $\{\psi_n\}$ are orthonormal, so that

$$\frac{1}{V_1} \int_{\mathcal{V}_1} \psi_m(\boldsymbol{x})\psi_n(\boldsymbol{x})d\boldsymbol{x} = \delta_{mn}, \tag{13.194}$$

and therefore the eigenfunction coefficients are given by

$$a_n = \frac{1}{V_1} \int_{\mathcal{V}_1} \psi_n(\boldsymbol{x})d\boldsymbol{x}. \tag{13.195}$$

Recall that

$$V_1 = \phi_1 V \tag{13.196}$$

is the *total pore volume*. Because the set $\{\psi_n\}$ is complete, we also have

$$\sum_{n=1}^{\infty} a_n^2 = 1. \tag{13.197}$$

The survival probability $S(t)$ in terms of $c(\boldsymbol{x}, t)$ is defined by the relation

$$S(t) = \frac{1}{V_1} \int_{\mathcal{V}_1} \frac{c(\boldsymbol{x}, t)}{c_o} d\boldsymbol{x}. \tag{13.198}$$

This quantity gives the fraction of Brownian particles that survive until time t; clearly, $S(0) = 1$. Substitution of (13.189) into (13.198) gives

$$S(t) = \sum_{n=1}^{\infty} a_n^2 e^{-t/T_n} . \tag{13.199}$$

The survival probability is depicted in Figure 13.12 for partially absorbing traps ($\kappa > 0$). It is a monotonically decreasing function of time; physically, a Brownian particle is more likely to get trapped as time progresses.

Remarks:

1. Interestingly, the problems described above have a direct connection to nuclear magnetic resonance (NMR) measurements in fluid-saturated porous media (Brownstein and Tarr 1979, Banavar and Schwartz 1987, Wilkinson, Johnson and Schwartz 1991). The characteristic times involved in the decay of nuclear magnetization are related to the pore size because of enhanced relaxation at the pore–solid interface. Therefore, NMR is a powerful noninvasive technique to study the microstructure and physical properties of fluid-saturated porous media. The equations governing the decay of the magnetization density $m(\boldsymbol{x}, t)$ (along a particular direction) are precisely (13.187) and (13.188) with $c(\boldsymbol{x}, t)$ and c_o replaced by $m(\boldsymbol{x}, t)$ and m_o, respectively. The dimensionless volume-integrated magnetization $M(t)/M_o$ ($M_o = m_o V_1$) is simply what we have referred to as the survival probability $S(t)$ given by (13.198), i.e.,
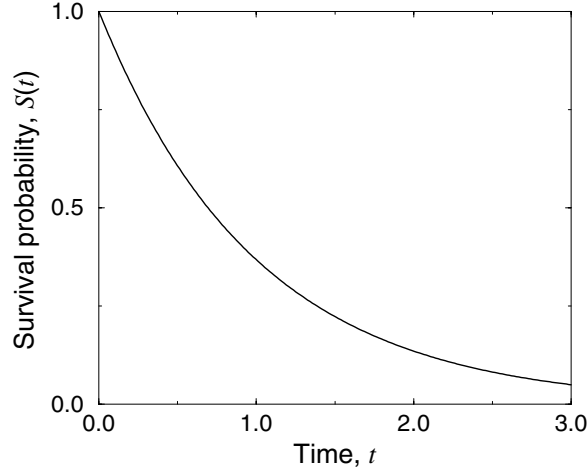
Figure 13.12 A schematic of the survival probability $S(t)$ versus time t for $\kappa > 0$.

$$S(t) = \frac{M(t)}{M_o}. \tag{13.200}$$

The net magnetization $M(t)$ is usually the quantity of principal interest in an NMR experiment. The survival probability has been computed for transport exterior to periodic arrays of spherical traps (Torquato and Kim 1992).

2. Ultimately, we will pass to the limit $V_1, V \to \infty$. In this limit, ergodicity enables us to equate ensemble and volume averages of some stochastic function $f(x)$ so that

$$\langle f \rangle = \lim_{V \to \infty} \frac{1}{V} \int f(x) dx. \tag{13.201}$$

The volume integrals (13.194), (13.195), and (13.198) become, respectively,

$$\frac{1}{\phi_1} \langle \psi_m \psi_n \rangle = \delta_{mn}, \tag{13.202}$$

$$a_n = \frac{1}{\phi_1} \langle \psi_n \rangle, \tag{13.203}$$

and

$$S(t) = \frac{1}{\phi_1} \left\langle \frac{c(x,t)}{c_o} \right\rangle. \tag{13.204}$$

Moreover, the spectrum $n(T)$ of the Laplace operator is no longer discrete but continuous, and so sums are replaced by integrals. For example, the series representation (13.199) of the survival probability $S(t)$ is replaced by

$$S(t) = \int_0^\infty n(T) e^{-t/T} dT.$$

3. The long-time behavior of the survival probability $S(t)$ is intimately connected to fluctuations in the pore size. The largest, or principal, relaxation time T_1 (inversely proportional to the smallest eigenvalue λ_1) is determined by the largest pores in the system. Therefore, when fluctuations in the pore size exist that are on the order of the system size, T_1 will diverge to infinity in the infinite-volume limit, and the associated spectrum will be continuous. The corresponding density of states near $\lambda_1 = 0$ is known as the "Lifshitz spectrum" in the theory of disordered systems (Lifshitz, Gredeskul and Pastur 1988). The associated survival probability becomes a stretched exponential, i.e., has the form $\exp[-a\, t^{d/(d+2)}]$ in d dimensions as $t \to \infty$ (Donsker and Varadhan 1975, Lifshitz et al. 1988).

13.7.2 Relationship Between Survival and Relaxation Times

Torquato and Avellaneda (1991) have shown that the mean survival time τ is bounded from above and below in terms of the principal relaxation T_1. Indeed, τ is related to the entire spectrum of the relaxation times (i.e., eigenvalues) or, equivalently, to the area under the survival probability curve $S(t)$. Thus, τ is a *simple but robust parameter* that describes the decay process. These statements are given in the form of two theorems and a corollary.

Theorem 13.2 *For random porous media of arbitrary microstructure at porosity ϕ_1, the following relation holds:*

$$\tau = \sum_{n=1}^{\infty} a_n^2 T_n, \tag{13.205}$$

where the a_n are the averages of the eigenfunctions ψ_n given by (13.203).

This theorem was proved by Torquato and Avellaneda (1991) by taking the Laplace transforms of (13.187) and (13.188) in time and recognizing that the transform of c evaluated at $s = 0$ (where s is the Laplace-transform variable) is trivially related to the steady-state concentration field u that solves (13.154) and (13.155). This proof is very similar to the one used to prove the analogous Theorem 23.6 involving the fluid permeability.

Corollary 13.1 *The mean survival time is also expressible as an integral over the survival probability as follows:*

$$\tau = \int_0^{\infty} S(t)dt. \tag{13.206}$$

This is easily proved by integrating relation (13.199) over all times and using Theorem 13.2.

Theorem 13.3 *For random porous media of arbitrary microstructure at porosity ϕ_1, the mean survival time τ is bounded from above and below in terms of the principal relaxation time T_1 as follows:*

$$a_1^2 T_1 \leq \tau \leq T_1. \tag{13.207}$$

This theorem follows from elementary properties of the eigenvalues (Torquato and Avellaneda 1991) and Theorem 13.2.

Remarks:
1. The aforementioned corollary and upper bound are valid whether the spectrum is discrete or continuous, and hence they hold for ergodic media.
2. The relaxation times are easy to evaluate for diffusion occurring inside certain simple domains. For example, in the case of transport interior to three-dimensional spherical pores of radius a (Torquato and Avellaneda 1991), the principal relaxation time T_1 obeys the following exact asymptotic expressions:

$$T_1 \sim \frac{a}{3\kappa} + \frac{a^2}{15\mathcal{D}} + \frac{17a^3\kappa}{525\mathcal{D}^2}, \qquad \frac{\kappa a}{\mathcal{D}} \ll 1, \tag{13.208}$$

$$T_1 \sim \frac{a^2}{\pi^2\mathcal{D}} + \frac{2a}{\pi^2\kappa}, \qquad \frac{\kappa a}{\mathcal{D}} \gg 1. \tag{13.209}$$

Comparing these results to the exact result $\tau = a^2/(15\mathcal{D}) + a/(3\kappa)$ for the survival time, as obtained from (16.83) with $d = 3$, reveals that the upper bound of Theorem 13.3 is very sharp for this simple pore geometry in both the diffusion-controlled and reaction-controlled regimes. This result suggests that the bound may be sharp for more general porous media, provided that they possess a narrow range of pore sizes.
3. Interestingly, Sapoval, Russ, Korb and Petit (1996) have computed the diffusion relaxation times for transport inside certain fractal pores.

13.8   Time-Dependent Flow Problem

In time-dependent flow, the key macroscopic properties are the so-called viscous relaxation times, which reflect information about the pore topology. Below we describe the basic equations and show an interesting connection to the steady-state *conduction* problem (Avellaneda and Torquato 1991).

13.8.1   Basic Equations

Consider the unsteady Stokes equations for the fluid velocity vector field $v(x,t)$ at position x and time t in $\mathcal{V}_1$:

$$\frac{\partial v}{\partial t} = -\nabla\left(\frac{p}{\rho}\right) + v\Delta v + v_0 e\delta(t) \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.210}$$

$$\nabla \cdot v = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.211}$$

$$v = 0 \qquad \text{on } \partial\mathcal{V}(\omega). \tag{13.212}$$

Here $p(x, t)$ is the pressure, ρ is the constant fluid density, ν is the kinematic viscosity, υ_0 is a constant speed, e is an arbitrary unit vector in the direction of the applied field, and $\delta(t)$ is the Dirac delta function. It will be implicit in all of the ensuing discussion that we assume a zero-traction condition at the boundary of $\mathcal{V}$.

The solution of (13.210)–(13.212) can be expressed as a sum of normal modes as follows:

$$\frac{\upsilon(x, t)}{\upsilon_0} = \sum_{n=1}^{\infty} b_n e^{-t/\Theta_n} \Psi_n(x), \tag{13.213}$$

where the vector eigenfunctions Ψ_n satisfy

$$\Delta \Psi_n + \nabla Q_n = -\epsilon_n \Psi_n \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.214}$$

$$\nabla \cdot \Psi_n = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.215}$$

$$\Psi_n = 0 \qquad \text{on } \partial \mathcal{V}(\omega). \tag{13.216}$$

Here the $\Theta_n = 1/(\nu \epsilon_n)$ are viscous relaxation times, and so the nth eigenvalue ϵ_n has dimensions of $(\text{length})^{-2}$. The functions Q_n in (13.214) are the corresponding pressures. The eigenfunctions Ψ_n are orthonormal, so that

$$\frac{1}{V_1} \int_{\mathcal{V}_1} \Psi_m(x) \cdot \Psi_n(x) dx = \delta_{mn}, \tag{13.217}$$

and the eigenfunction expansion coefficients are given by

$$b_n = \frac{1}{V_1} \int_{\mathcal{V}_1} e \cdot \Psi_n(x) dx. \tag{13.218}$$

Here $V_1 = \phi_1 V$ denotes the total pore volume.

Note that the set of orthonormal eigenfunctions Ψ_n is complete in the closed subspace of square integrable divergence-free fields having zero normal component on $\partial \mathcal{V}$ (Temam 1979). According to the classical Hodge decomposition (Temam 1979), we can express the constant unit vector e as the sum of a solenoidal field, with vanishing normal component on the pore–solid interface, and the gradient of a potential, as follows:

$$e = E + \nabla \varphi. \tag{13.219}$$

Here E is a dimensionless field satisfying

$$\nabla \cdot E = 0 \qquad \text{in } \mathcal{V}_1(\omega), \tag{13.220}$$

$$E \cdot n = 0 \qquad \text{on } \partial \mathcal{V}_1(\omega), \tag{13.221}$$

where n is the unit outward normal from the pore region. Relation (13.219) implies that

$$\nabla \times E = 0 \qquad \text{in } \mathcal{V}_1(\omega). \tag{13.222}$$

We observe that the field E then solves the corresponding electric conduction problem for a porous medium filled with a conducting fluid of conductivity σ_1 and having an

insulating solid phase. Hence, E can be physically interpreted as a scaled electric field, i.e., the actual electric field divided by the magnitude of the ensemble-averaged electric field. The field E is related to the scaled effective conductivity of the porous medium σ_e/σ_1 by the energy representation formula (see Theorem 14.1)

$$\sigma_e/\sigma_1 = F^{-1} = \langle E \cdot E \rangle. \tag{13.223}$$

Here $F \equiv \sigma_1/\sigma_e$ is the dimensionless inverse effective conductivity, referred to as the *formation factor*, and angular brackets denote an ensemble average. For statistically homogeneous media, ergodicity enables us to equate ensemble averages with volume averages, and therefore the average of an arbitrary stochastic function $f(x)$ is defined by (13.201). Substitution of (13.219) into (13.218) yields, after integration by parts,

$$b_n = \frac{1}{V_1} \int_{\mathcal{V}_1} E(x) \cdot \Psi_n(x) dx$$
$$= \frac{1}{\phi_1} \langle E \cdot \Psi_n \rangle. \tag{13.224}$$

Therefore, the coefficients b_n coincide with the coefficients of the normal mode expansion of the dimensionless field E in the orthonormal set of solenoidal eigenfunctions $\{\Psi_n\}$. Since the Ψ_n are complete in the aforementioned subspace, we have

$$\sum_{n=1}^{\infty} b_n \Psi_n = E \tag{13.225}$$

and

$$\sum_{n=1}^{\infty} b_n^2 = \frac{1}{\phi_1} \langle E \cdot E \rangle = \frac{1}{\phi_1} \frac{\sigma_e}{\sigma_1} = \frac{1}{F\phi_1}. \tag{13.226}$$

The product $F\phi_1$ is referred to as the *tortuosity*. The completion formula (13.226) will prove very useful in deriving cross-property relations between fluid permeability and effective diffusion parameters.

To summarize, we have shown the remarkable result that *the response of the Stokes fluid to a unit applied pressure gradient e is identical to the response obtained if e is replaced by E, the dimensionless electric field*. The reason for this is that in steady state, the gradient of the potential, $\nabla\varphi$, in the Hodge decomposition of e corresponds to a pressure fluctuation that does not affect the velocity field.

13.8.2   Relationship Between Permeability and Relaxation Times

Just as the steady-state mean survival time can be related to the diffusion relaxation times T_n, the steady-state permeability k can be related to the viscous relaxation times Θ_n. However, unlike the former case, the latter connection also involves a different effective property of the porous medium, namely, the effective conductivity. Accordingly, this *cross-property* relation will be derived in Chapter 23.