Diffusion in Random Media

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Abstract

We present a survey of homogenization methods for diffusion equations with periodic and random diffusivity.

Contents

1 Introduction

Diffusion in heterogeneous media can frequently be described by its *effective* behavior. This means that there is a homogeneous medium, the effective medium, whose diffusive properties are close to those of the real medium when measured on long space-time scales. A process of averaging or *homogenization* takes place so that the complicated small scale structure of the material is replaced by an asymptotically equivalent homogeneous structure.

Calculating the effective properties of complex materials is a basic problem in Physics to which Maxwell, Rayleigh, Lorentz, Debye and many other distinguished scientists have contributed. Homogenization as a mathematical problem regarding the asymptotic behavior of solutions of partial differential equations with rapidly changing coefficients became established in the nineteen seventies. Its early form [1, 2] did not exploit the idea of multiple scale analysis. This was done in [3] for periodic structures and more recently in [4] and [5]. The general theory of Γ convergence, started by DeGiorgi and Spagnolo, is presented in [6].

The purpose of this article is to give a brief and self contained presentation of homogenization in *random* media. The passage from periodic to random media is not so well understood because the multiple scale analysis, which is simple and very effective in periodic structures, is not so simple in random media. This, in particular, makes computational issues much more involved for random media. The extension of the basic analysis of [3] to random media was given in [7] and [8]. Of course, homogenization is only a small part of the story of understanding the effective behavior of complex materials. It tells us in a mathematically precise way that the replacement of the original equation by one with constant coefficients is a valid approximation in a certain limit. It does not tell us how to compute the effective coefficients. We present only a few methods and ideas that come into play in the determination of the effective coefficients: the Maxwell-Claussius-Mossotti formula (section 3.2), the Rayleigh-Hasimoto method (section 3.4) and conductivity in a region with holes (section 3.5).

2 One-Dimensional Conductors

2.1 Effective conductivity

Let $D(x)$, $x \in \mathbf{R}^1$, denote the conductivity and $u(x)$ the temperature of a conductor. If a unit temperature gradient is imposed on an interval $[-N, N]$ occupied by the conductor, the temperature is determined by solving the equation

$$\frac{d}{dx}\left(D(x)\frac{du(x)}{dx}\right) = 0 \ , \qquad \text{in} \qquad [-N, N] \tag{2.1}$$

with

$$u(-N) = -N \ , \qquad u(+N) = N \ . \tag{2.2}$$

The average heat flow per unit temperature gradient is the effective conductivity of the material

$$D_N = \frac{1}{2N}\int_{-N}^{N} D(x)\frac{du(x)}{dx}\, dx \tag{2.3}$$

In one-dimensional conductors the local heat flux Du_x is constant, as can be seen from (2.1), if there are no heat sources or sinks. Therefore the integral in (2.3) is unnecessary.

It is convenient however to adopt (2.3) as definition of effective conductivity. For the definition to make sense, the size $2N$ of the sample of the conductor must be much larger than the scale of variation of the local conductivity $D(x)$. It is therefore reasonable to try to find the limit of D_N as $N \to \infty$. If the limit exists we set

$$D^* = \lim_{N\to\infty} D_N \tag{2.4}$$

and call D^* the *effective* or *bulk* conductivity.

In one dimensional media the existence of the effective conductivity is easy to establish because we have an explicit expression for D_N. In fact, since Du_x is constant,

$$D_N = D(x)\, u_x(x)$$

and solving for u and applying the boundary conditions (2.2) we get

$$D_N = \left(\frac{1}{2N} \int_{-N}^{N} \frac{1}{D(x)}\, dx \right)^{-1} \tag{2.5}$$

It is assumed of course that $D(x)$ is positive so that (2.5) makes sense. If $D(x)$ is periodic of period 1 then

$$D^* = \lim_{N\to\infty} D_N = \left(\int_0^1 \frac{1}{D(x)}\, dx \right)^{-1} \tag{2.6}$$

which is the harmonic mean of the local conductivity. Similarly, if $D(x)$ is a stationary random process with[1]

$$E\left\{ \frac{1}{D(x)} \right\} < \infty$$

then the ergodic theorem [9] tells us that

$$D^* = \left(E\left\{ \frac{1}{D(x)} \right\} \right)^{-1} \tag{2.7}$$

It is easy to see that (2.7) is the correct result because the effective resistivity $(D^*)^{-1}$ is just the average resistivity of a continuum resistor network in series.

It is instructive to formulate the notion of effective conductivity in another equivalent form. Let

$$\epsilon = \frac{1}{N}$$

[1]Here $E\{\,\}$ denotes expectation or ensemble average.

and define

$$D^\epsilon(x) = D\left(\frac{x}{\epsilon}\right) \ , \qquad u^\epsilon(x) = u(\frac{x}{\epsilon}) \tag{2.8}$$

With this scaling, problem (2.1–2.2) becomes

$$(D^\epsilon(x)\, u_x^\epsilon(x))_x = 0 \quad \text{in} \quad [-1, 1] \tag{2.9}$$

with

$$u^\epsilon(-1) = 1 \ , \qquad u^\epsilon(+1) = 1 \ . \tag{2.10}$$

We can write the temperature $u^\epsilon(x)$ in the form

$$u^\epsilon(x) = x + \chi^\epsilon(x) \tag{2.11}$$

Then $\chi^\epsilon(x)$ satisfies

$$(D^\epsilon(1 + \chi_x^\epsilon))_x = 0 \ , \quad \text{in} \quad [-1, 1] \tag{2.12}$$

with

$$\chi^\epsilon(\pm 1) = 0 \ . \tag{2.13}$$

The function χ^ϵ represents the local difference in temperature that results when a unit temperature gradient is imposed. The effective conductivity is now given by

$$D^* = \lim_{\epsilon \downarrow 0} \frac{1}{2} \int_{-1}^{1} D^\epsilon(1 + \chi_x^\epsilon)\, dx \tag{2.14}$$

In the periodic case, $u^\epsilon(x) = x + \epsilon\chi(x/\epsilon)$ with $\chi(y)$ periodic with period one and satisfying

$$(D(y)(1 + \chi_y))_y = 0 \ . \tag{2.15}$$

The effective conductivity is given again by (2.6). The local filed χ is given by

$$\chi(y) = \int_0^y \left\{ \left(\int_0^1 \frac{1}{D(x)} dx \right)^{-1} \frac{1}{D(y)} - 1 \right\} dy \tag{2.16}$$

2.2 Homogenization

The main point of homogenization is that the above definition of effective conductivity contains more information than is immediately apparent. It tells us, for example, that if $f(x)$ is any smooth function the solution of the problem

$$-(D^\epsilon u_x^\epsilon)_x = f(x) \ , \qquad x \in O \tag{2.17}$$

with

$$u^\epsilon = 0 \quad \text{on} \quad \partial O \tag{2.18}$$

converges as $\epsilon \to 0$ to the solution $u(x)$ of the problem

$$-(D^* u_x)_x = f(x) \ , \qquad x \in O \tag{2.19}$$

with

$$u = 0 \quad \text{on} \quad \partial O \tag{2.20}$$

Here O is any interval on the line and ∂O is the set of its two end points. If $f(x)$ belongs to $L^2(O)$ so that

$$\int_O |f(x)|^2 \, dx < \infty \ , \tag{2.21}$$

$D^\epsilon(x) = D(x/\epsilon)$ with $D(y)$ periodic of period one and

$$0 < D_1 \leq D(y) \leq D_2 < \infty \ , \tag{2.22}$$

then $u^\epsilon \to u$ in the L^2 sense

$$\int_O |u^\epsilon(x) - u(x)|^2 \, dx \to 0 \tag{2.23}$$

as $\epsilon \to 0$.

The proof of this result is quite simple in one space dimension because we have an explicit solution for $u^\epsilon(x)$:

$$u^\epsilon(x) = c_1 \int_0^x \frac{1}{D^\epsilon(s)} \, ds - \int_0^x \frac{1}{D^\epsilon(s)} \int_0^s f(\sigma) \, d\sigma \, ds + c_2 \tag{2.24}$$

where c_1 and c_2 are constants (depending on ϵ) that are determined from the boundary conditions (2.18). From this formula we see that, in the periodic case, the convergence $u^\epsilon \to u$ will take place pointwise as well as in L^2, (2.23), if we have the following result.

Let $F(y, x)$ be a bounded function that is periodic in y of period 1 and a smooth function of x. Then

$$\lim_{\epsilon \downarrow 0} \int_\alpha^\beta F(\frac{x}{\epsilon}, x) \, dx = \int_\alpha^\beta \overline{F}(x) \, dx \tag{2.25}$$

where

$$\overline{F}(x) = \int_0^1 F(y, x) \, dy$$

There are many proofs of this result and it holds under much weaker conditions than those stated. But there is a very simple proof with the present hypotheses. Let

$$G(y,x) = \int_0^y \Big(F(z,x) - \overline{F}(x)\Big)\, dz \tag{2.26}$$

and note that $G(y,x)$ is a bounded (periodic) function of y and smooth in x. We now note that

$$\int_\alpha^\beta \Big[F(\frac{x}{\epsilon},x) - \overline{F}(x)\Big]\, dx = \epsilon\, G(\frac{\beta}{\epsilon},\beta) - \epsilon G(\frac{\alpha}{\epsilon},\alpha) - \epsilon \int_\alpha^\beta G_x(\frac{x}{\epsilon},x)\, dx \tag{2.27}$$

and since the right-hand side is $O(\epsilon)$ the result (2.25) follows. It is clear that the liberal regularity condition that we imposed yielded not only (2.25) but also an $O(\epsilon)$ estimate of the rate of convergence. The result (2.25) is true if $F(y,\cdot)$ is a bounded periodic function with values in $L^1(\alpha,\beta)$. It is also true in the stationary random case and in several dimensions. The random case will be discussed in section 4.1. The multidimensional periodic case is proved, in the smooth case, by constructing a vector function $G(y,x)$ such that

$$\nabla_y \cdot G(y,x) = F(y,x) - \overline{F}(x)$$

where ∇_y is the gradient with respect to the y variables. An application of the divergence theorem produces an identity like (2.27) and hence the multidimensional version of (2.25) follows.

We now apply (2.25) to the right side of (2.24). In the periodic case $D^\epsilon(x) = D(x/\epsilon)$ and, in view of (2.21) and (2.22), (2.25) applies. The limit is the explicit solution of (2.19) if we recall that D^* is the harmonic mean of $D(y)$ given by (2.6).

2.3 General homogenization

From the explicit solution (2.24) we can also see that the convergence (2.23) holds in much greater generality, not only in the periodic or stationary random case (discussed in section 3.1). Let $D^\epsilon(x)$ stand for an arbitrary sequence of measurable functions that satisfy

$$0 < D_1 \leq D^\epsilon(x) \leq D_2 < \infty \tag{2.28}$$

For example $D^\epsilon(x)$ may have the form $D(x, x/\epsilon, x/\epsilon^2, x/\epsilon^3)$ with $D(x,y,z,w)$ periodic in y,z,w, indicating that the small scale variations are associated with several different scales.

In general homogenization theory [6] we only know (2.28) and look for the weakest type of convergence that is compatible with the approximation (2.19) of (2.17). The effective conductivity D^* will not be a constant now and will be hard to characterize in general. In the one dimensional case we have the explicit solution (2.24) and so we know what we need to get D^*. If $1/D^\epsilon(x)$ converges weakly to $1/D^*(x)$ then we have convergence in L^2, as in (2.23). By weak convergence we mean that for any integrable function g in O

$$\int_O \frac{1}{D^\epsilon(x)} g(x)dx \to \int_O \frac{1}{D^*(x)} g(x)dx \tag{2.29}$$

as ϵ tends to zero.

2.4 Anomalous diffusion

If $D(x)$ in

$$\frac{d}{dx}\left(D(x)\frac{du(x)}{dx}\right) = 0 \ , \quad \text{in} \quad [-N,N]//u(-N) = -N \ , \qquad u(+N) = N \ . \tag{2.30}$$

is not stationary then the effective conductivity D_N

$$D_N = \frac{1}{2N}\int_{-N}^{N} D(x)\frac{du(x)}{dx}\,dx \tag{2.31}$$

will not have a limit as $N \to \infty$. This will be the case, for example, if $D(x) = e^{w(x)}$ where $w(x)$ is the standard Brownian motion process whose increments are stationary but it is not itself stationary. The anomalous behavior of D_N is best seen in the time domain for the diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial u(x,t)}{\partial x}\right) \ , \quad \text{in} \quad (-\infty,\infty) \tag{2.32}$$

with $u(x,0) = \delta(x)$, the delta function with unit mass at the origin. In the case of stationary $D(x)$ it is easy to see using Laplace transforms that as t goes to infinity

$$\frac{1}{t}\int_{-\infty}^{\infty} x^2 u(x,t)dx \to D^* \tag{2.33}$$

which says that the mean square displacement of the diffusing particle is asymptotically linear in time and the effective diffusivity D^* is the rate constant. When $D(x) = e^{w(x)}$ then

$$\int_{-\infty}^{\infty} x^2 u(x,t)dx \approx O(\log^4 t) \tag{2.34}$$

in a suitable sense as t tends to infinity, first studied by Sinai [10] for the equivalent discrete model. Thus, when the microscopic diffusivity is nonstationary the mean square displacement is much smaller than that for normal diffusion. The diffusing particle has been effectively localized, much like waves localize in one dimensional random media. A recent study of diffusion localization is [11].

3 Multidimensional Diffusion

3.1 Periodic homogenization

3.1.1 The multiple scale expansion

In several dimensions we need a general way to get the the approximation by an equation with effective coefficients. To introduce the method of multiple scales for problems with periodic coefficients we consider the convection-reaction-diffusion equation

$$\frac{\partial u}{\partial t} + \mathbf{v}(\mathbf{x}) \cdot \nabla u = \nabla \cdot (D(\mathbf{x}) \nabla u) + a(\mathbf{x}) u \tag{3.1}$$

$$u(0, \mathbf{x}) = f(\varepsilon \mathbf{x}) \tag{3.2}$$

Here $\varepsilon > 0$ is a small parameter indicating that the initial concentration (or temperature) is slowly varying compared to the variation of the coefficients in (3.1), which are: the convective velocity $\mathbf{v}$, the diffusivity D and the reaction rate a. All three are assumed to be periodic functions with period one in each direction and $D(\mathbf{x})$ is strictly positive and bounded. All three are assumed to be smooth (for the elementary demonstration of this section) and the initial concentration is also assumed to be smooth and have compact support. To fix ideas we consider the three dimensional problem.

First we pass to macroscopic coordinates in (3.1), (3.2) by replacing $t \to t/\varepsilon^2$ and $\mathbf{x} \to \mathbf{x}/\varepsilon$. In these coordinates (3.1) and (3.2) become

$$\frac{\partial u}{\partial t} + \frac{1}{\varepsilon} \mathbf{v}\left(\frac{\mathbf{x}}{\varepsilon}\right) \cdot \nabla u = \nabla \cdot \left(D\left(\frac{\mathbf{x}}{\varepsilon}\right) \nabla u\right) + \frac{1}{\varepsilon^2} a\left(\frac{\mathbf{x}}{\varepsilon}\right) u, \tag{3.3}$$

$$u(0, \mathbf{x}) = f(\mathbf{x}) \tag{3.4}$$

The key in the multiple scale analysis is to look for $u(t, \mathbf{x})$ in the form $w\left(t, \mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right)$ and in the analysis treat $w(t, \mathbf{x}, \mathbf{y})$ as if $\mathbf{x}$ and $\mathbf{y}$ were independent variables, which of course they are not but $w\left(t, \mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right)$ captures the essential features of $u(t, \mathbf{x})$. More specifically, we try to find $w(t, \mathbf{x}, \mathbf{y})$, with unit periodic dependence in $\mathbf{y}$, that satisfies the **expanded** equation

$$
\begin{aligned}
\frac{\partial w}{\partial t} &+ \frac{1}{\varepsilon}\mathbf{v}(\mathbf{y}) \cdot \left(\nabla_x + \frac{1}{\varepsilon}\nabla_y\right) w \\
&= \left(\nabla_x + \frac{1}{\varepsilon}\nabla_y\right) \cdot \left(D(\mathbf{y})(\nabla_x + \frac{1}{\varepsilon}\nabla_y)w\right) + \frac{1}{\varepsilon^2}a(\mathbf{y})w \\
w(0, \mathbf{x}, \mathbf{y}) &= f(\mathbf{x})
\end{aligned} \tag{3.5}
$$

Grouping terms according to powers of ε we get

$$
\begin{aligned}
&\frac{1}{\varepsilon^2}[\nabla_y \cdot (D\nabla_y w) - \mathbf{v} \cdot \nabla_y w + aw] \\
&+\frac{1}{\varepsilon}[\nabla_x \cdot (D\nabla_y w) + \nabla_y \cdot (D\nabla_x w) - \mathbf{v} \cdot \nabla_x w] \\
&+[\nabla_x \cdot (D\nabla_x w) - w_t] = 0
\end{aligned} \tag{3.6}
$$

Normally the next step is to assume that w has a power series expansion in ε

$$
w = w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \ldots \tag{3.7}
$$

and after inserting this expansion in (3.6) get equations for w_0, w_1, w_2, etc. In many situations, for example for (3.6), this is too simple and will not work. If there is no reaction so that $a \equiv 0$ in (3.3) and if $\mathbf{v}$ is incompressible ($\nabla \cdot \mathbf{v} = 0$) and has mean zero (average over the unit period cell is zero) then the direct expansion (3.7) will work fine. In general the reaction rate induces its own macroscopic concentration balance and compressibility with overall bulk convection will also affect the long-time behavior. We therefore introduce a scalar λ and a vector $\mathbf{M}$ in (3.6), which we will determine later, and rewrite it in the form

$$
\begin{aligned}
&\frac{1}{\varepsilon^2}[\nabla_y \cdot (D\nabla_y w) - \mathbf{v} \cdot \nabla_y w + aw - \lambda w] \\
&+\frac{1}{\varepsilon}[\nabla_x \cdot (D\nabla_y w) + \nabla_y \cdot (D\nabla_x w) - \mathbf{v} \cdot \nabla_x w + \mathbf{M} \cdot \nabla_x w] \\
&+\left[\nabla_x \cdot (D\nabla_x w) - \frac{\partial w}{\partial t} + \frac{\lambda}{\varepsilon^2}w - \frac{M}{\varepsilon}\nabla_x w\right] = 0
\end{aligned} \tag{3.8}
$$

Nothing has changed, of course, because the terms inserted are removed in the last line in (3.8). The fact that ε-dependent terms appear out of place in (3.8) is an essential part of the analysis and we will discuss it further later. For now the ε-dependent terms in the last line in (3.8) will be regarded as comparable to the other 0(1) terms.

With this understanding, we insert the expansion (3.7) into (3.8) and get the following sequence of problems.

$$\nabla_y \cdot (D\nabla_y w_0) - \mathbf{v} \cdot \nabla_y w_0 + a w_0 - \lambda w_0 = 0 \tag{3.9}$$

$$\begin{aligned} \nabla_y \;\cdot\; & (D\nabla_y w_1) - \mathbf{v} \cdot \nabla_y w_1 + a w_1 - \lambda w_1 \\ & + \nabla_x \cdot (D\nabla_y w_0) + \nabla_y \cdot (D\nabla_x w_0) - \mathbf{v} \cdot \nabla_x w_0 + \mathbf{M} \cdot \nabla_x w_0 = 0 \end{aligned} \tag{3.10}$$

$$\begin{aligned} \nabla_y \;\cdot\; & (D\nabla_y w_2) - \mathbf{v} \cdot \nabla_y w_2 + a w_2 - \lambda w_2 \\ & + \nabla_x \cdot (D\nabla_y w_1) + \nabla_y \cdot (D\nabla_x w_1) - \mathbf{v} \cdot \nabla_x w_1 + \mathbf{M} \cdot \nabla_x w_1 \\ & + \nabla_x \cdot (D\nabla_x w_0) - \frac{\partial w_0}{\partial t} + \frac{\lambda}{\varepsilon^2} w_0 - \frac{1}{\varepsilon}\mathbf{M} \cdot \nabla_x w_0 = 0 \end{aligned} \tag{3.11}$$

Consider first (3.9) in which we separate $w_0 = w_0(t, \mathbf{x}, \mathbf{y})$ into the product

$$w_0 = \overline{u}(t, \mathbf{x})\phi(\mathbf{y}) \tag{3.12}$$

so that (3.9) becomes an equation for $\phi(\mathbf{y})$ over the period cell

$$\nabla_y \cdot (D\nabla_y \phi) - \mathbf{v} \cdot \nabla_y \phi + a\phi - \lambda\phi = 0 \tag{3.13}$$

and $\overline{u}$ drops out because (3.9) has no $\mathbf{x}$ or t derivatives. It will be determined later. We concentrate therefore on (3.13) and it now becomes clear why λ was inserted in (3.8). Equation (3.13) is an eigenvalue problem. In fact, for an elliptic equation like (3.13) over a period cell there is a largest eigenvalue $\lambda < \infty$ and the corresponding eigenfunction $\phi(\mathbf{y})$ is positive (and periodic). This is an important fact that is not immediately obvious because (3.13) is not selfadjoint. If the reaction rate $a \equiv 0$ then $\lambda = 0$ and $\phi \equiv 1$ are the maximal eigenvalue and eigenfunction for (3.13). Depending on the sign of a the eigenvalue λ can be positive, negative or zero in general. It is an isolated eigenvalue since the resolvent of the operator in (3.13) is compact. The positivity of ϕ is a consequence of the maximum principle for the second order operator in (3.13). We also need the equation adjoint to (3.13)

$$\nabla_y \cdot (D\nabla_y \psi) + \nabla \cdot (\mathbf{v}\psi) + a\psi - \lambda\psi = 0 \tag{3.14}$$

which has the same eigenvalue λ as (3.13) and a positive eigenfunction $\psi(\mathbf{y})$. We normalize ϕ and ψ by

$$\int_0^1\int_0^1\int_0^1 \phi(\mathbf{y})\psi(\mathbf{y})d\mathbf{y} = 1 \ ,$$
$$\int_0^1\int_0^1\int_0^1 \psi(\mathbf{y})d\mathbf{y} = 1 \tag{3.15}$$

We consider next (3.10) which is an inhomogeneous version of (3.9) for $w_1(t,\mathbf{x},\mathbf{y})$. The $(t,\mathbf{x})$ variables are parameters in this equation. The solvability condition for (3.10) determines the vector $\mathbf{M}$. Multiplying (3.10) by ψ, integrating over the unit cell, integrating by parts, and using (3.14) we get

$$\int_0^1\int_0^1\int_0^1 \psi(\mathbf{y})[\nabla_x\cdot(D\nabla_y\overline{u}\phi)+\nabla_y\cdot(D\nabla_x\overline{u}\phi)$$
$$-\mathbf{v}\cdot\nabla_x\overline{u}\phi+\mathbf{M}\cdot\nabla_x\phi\overline{u}\,]\,d\mathbf{y} = 0 \ .$$

Since $\overline{u}=\overline{u}(t,\mathbf{x})$ we can rewrite this in the form

$$\mathbf{M} = \int_0^1\int_0^1\int_0^1 [\psi(\mathbf{y})\mathbf{v}(\mathbf{y})\phi(\mathbf{y})+D(\mathbf{y})\left(\phi(\mathbf{y})\nabla\psi(\mathbf{y})-\psi(\mathbf{y})\nabla\phi(\mathbf{y})\right)]\,d\mathbf{y} \tag{3.16}$$

where we also use the normalization (3.15). With $\mathbf{M}$ so determined (3.10) is solvable in the form

$$w_1 = \nabla_x\overline{u}\cdot\boldsymbol{\chi}\phi \tag{3.17}$$

with the periodic vector function $\boldsymbol{\chi}(\mathbf{y})$ satisfying

$$\nabla\cdot(D\nabla\boldsymbol{\chi})-\mathbf{v}\cdot\nabla\boldsymbol{\chi}+2D\nabla\boldsymbol{\chi}\cdot\nabla\log\phi+2D\nabla\log\phi+\nabla D-(\mathbf{v}-\mathbf{M})=0 \tag{3.18}$$

The solution $\boldsymbol{\chi}$ is determined up to an additive multiple of ϕ which we choose to be zero since it does not affect the way $\overline{u}(t,\mathbf{x})$ is determined next.

We now consider (3.11) which is again an inhomogeneous version of (3.9) and its solvability condition determines $\overline{u}$. Using (3.14) and the normalization (3.15) we find that $\overline{u}$ satisfies the homogenized convection diffusion equation.

$$\frac{\partial\overline{u}}{\partial t}+\frac{1}{\varepsilon}\mathbf{M}\cdot\nabla_x\overline{u} = \sum_{i,j=1}^{3} D^*_{ij}\frac{\partial^2\overline{u}}{\partial x_i\partial x_j}+\frac{\lambda}{\varepsilon^2}\overline{u} \tag{3.19}$$
$$\overline{u}(0,\mathbf{x}) = f(\mathbf{x}) \tag{3.20}$$

We will discuss the initial condition for (3.19) after the effective diffusivity matrix D^* is given in a convenient form. The solvability condition gives, at first,

$$\begin{aligned}
D^*_{ij} = \int_0^1 \int_0^1 \int_0^1 \Big\{ & D(\mathbf{y})\psi(\mathbf{y})\phi(\mathbf{y})\frac{\partial \chi_j(\mathbf{y})}{\partial y_i} \\
& + D(\mathbf{y})\chi_j(\mathbf{y}) \left(\psi(\mathbf{y})\frac{\partial \phi(\mathbf{y})}{\partial y_i} - \phi(\mathbf{y})\frac{\partial \psi(\mathbf{y})}{\partial y_j} \right) - \left(v_i(\mathbf{y}) - M_i\right)\chi_j \cdot \phi(\mathbf{y})\psi(\mathbf{y}) \\
& + D(\mathbf{y})\delta_{ij}\phi(\mathbf{y})\psi(\mathbf{y}) \Big\} \, d\mathbf{y}
\end{aligned} \tag{3.21}$$

Note however that only the symmetric part of (3.21) enters in (3.19). This is an important observation in simplifying (3.21). For the simplification, we first multiply (3.18) by $\phi\psi\boldsymbol{\chi}$ and integrate. Since $\boldsymbol{\chi}$ is a vector we actually multiply the i-th equation (3.18) by $\phi\psi\chi_j, \ i,j = 1,2,3$. This gives an expression for

$$\int_0^1 \int_0^1 \int_0^1 \left(v_i(\mathbf{y}) - M_i\right)\chi_j(\mathbf{y})\phi(\mathbf{y})\psi(\mathbf{y})d\mathbf{y}$$

which we insert in (3.21). We use the defining equation (3.13) in this step. The result is a complicated expression which we simplify further by considering only the symmetric part and by using the identity

$$\nabla \cdot (\phi D \nabla \psi - \psi D \nabla \phi + \mathbf{v}\phi\phi) = 0 \tag{3.22}$$

which we get by multiplying (3.14) by ϕ, (3.13) by ψ and subtracting. After this simplification we get

$$D^*_{ij} = \int_0^1 \int_0^1 \int_0^1 \phi(\mathbf{y})\psi(\mathbf{y})D(\mathbf{y}) \sum_{\ell=1}^{3} \left(\delta_{i\ell} + \frac{\partial \chi_i(\mathbf{y})}{\partial y_\ell}\right) \left(\delta_{j\ell} + \frac{\partial \chi_j(\mathbf{y})}{\partial y_\ell}\right) d\mathbf{y} \tag{3.23}$$

which shows clearly that D^* is a positive definite matrix.

3.1.2 Initial layer

It remains to discuss the initial values that go into the homogenized problem (3.19). First we look at what has been accomplished so far. We have determined completely the first term in the multiple scales expansion (3.7) of w. This means that since $\mathbf{y} = \mathbf{x}/\varepsilon$ we have an approximation of the solution of (3.3), (3.4) in the form

$$u(t,\mathbf{x}) \sim \overline{u}(t,\mathbf{x})\phi\left(\frac{\mathbf{x}}{\varepsilon}\right) + O(\varepsilon), \quad t > 0 \tag{3.24}$$

with ϕ determined by the eigenvalue problem (3.13) and $\overline{u}$ the solution of (3.19). Note that $\overline{u}$ depends on the parameter $\varepsilon > 0$ but has *constant* coefficients. The mean convection velocity $\mathbf{M}$ is given by (3.16), the mean reaction rate λ is the eigenvalue in (3.13) and effective diffusivity D^* is given by (3.23) after the *cell* problem (3.18) is solved.

From this summary it is clear that (3.24) is incompatible with the initial values (3.4) since the right side of (3.24) gives at $t = 0$, $f(\mathbf{x})\phi\left(\frac{\mathbf{x}}{\varepsilon}\right)$, in view of (3.20). Note first that we carefully limited (3.24) to $t > 0$; it is not valid uniformly all the way to $t = 0$. To see why (3.20) is the right initial condition for the homogenized problem we argue in the following manner.

Let $\tau = t/\varepsilon^2$ be the microscopic time scale. The principal term in the multiple scale space-time expansion of (3.3) does not satisfy now the time homogeneous problem (3.9) but

$$\frac{\partial \widetilde{w}_0}{\partial \tau} = \nabla_y \cdot (D \nabla_y \widetilde{w}_0) - \mathbf{v} \cdot \nabla_y \widetilde{w}_0 + a\widetilde{w}_0 - \lambda \widetilde{w}_0 \tag{3.25}$$

with $\widetilde{w}_0(0, \mathbf{y}, \mathbf{x}) = f(\mathbf{x})$ as initial condition. Of course in (3.25) the variable $\mathbf{x}$ is just a parameter and (3.7) is the limiting form of (3.25) as $\tau \to \infty$. To get the correct form of the initial value for $\overline{u}(t, \mathbf{x})$ we must have the $t = 0$ limit of w_0. In the language of matched asymptotic expansions we must have the inner limit of the outer expansion equal the outer limit of the initial layer expansion. It is easy to see that as $\tau \to \infty$

$$\begin{aligned} \widetilde{w}_0(\tau, \mathbf{x}, \mathbf{y}) &\sim \phi(\mathbf{y}) \int_0^1 \int_0^1 \int_0^1 \psi(\mathbf{y}) f(\mathbf{x}) d\mathbf{y} \\ &= \phi(\mathbf{y}) f(\mathbf{x}) \end{aligned} \tag{3.26}$$

because of the normalization condition (3.15). From (3.12) we see that

$$w_0(0, \mathbf{x}, \mathbf{y}) = \overline{u}(0, \mathbf{x}) \phi(\mathbf{y}) \tag{3.27}$$

Therefore we must have $\overline{u}(0, \mathbf{x}) = f(\mathbf{x})$ which is (3.20).

Note that if the initial condition (3.4) is replaced by

$$u(0, \mathbf{x}) = f\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) \tag{3.28}$$

then (3.26) becomes

$$\widetilde{w}_0(t, \mathbf{x}, \mathbf{y}) \sim \phi(\mathbf{y}) \int_0^1 \int_0^1 \int_0^1 \psi(\mathbf{y}) f(\mathbf{x}, \mathbf{y}) d\mathbf{y} \tag{3.29}$$

and hence instead of (3.20) we have for (3.19) the initial condition

$$\overline{u}(0,\mathbf{x}) = \int_0^1 \int_0^1 \int_0^1 \psi(\mathbf{y}) f(\mathbf{x},\mathbf{y}) d\mathbf{y} \tag{3.30}$$

3.1.3 Interpretation of homogenization and the cell problem

What have we achieved with the multiple scale expansion? We have shown formally, and it is not hard in the periodic case to give a full proof based on the expansion, that the solution of (3.3,3.4) behaves like

$$u(t,\mathbf{x}) \sim \bar{u}(t,\mathbf{x})\phi(\frac{\mathbf{x}}{\varepsilon}) \tag{3.31}$$

with $\phi(\mathbf{y})$ the (periodic) local equilibrium-reaction density satisfying (3.13) and $\bar{u}(t,\mathbf{x})$ satisfying the homogeneous diffusion equation (3.19). We can solve this equation explicitly and $\bar{u}$ depends on ε. The effective reaction rate λ/ε^2 is large, if λ is not close to zero, and the effective velocity $\mathbf{M}/\varepsilon$ is also large compared to the effective diffusivity D^*. Let $U(t,\mathbf{x})$ satisfy

$$\frac{\partial U}{\partial t} = \sum_{i,j=1}^{3} D^*_{ij} \frac{\partial U}{\partial x_i \partial x_j} \tag{3.32}$$

$$U(0,\mathbf{x}) = f(\mathbf{x}) \tag{3.33}$$

Then

$$\bar{u}(t,\mathbf{x}) = e^{\lambda t/\varepsilon^2} U(t,\mathbf{x} - \frac{\mathbf{M}t}{\varepsilon}) \tag{3.34}$$

so that the solution of the original problem (3.3, 3.4) is close to U for small ε if the reaction and translation are removed

$$\frac{e^{-\lambda t/\varepsilon^2}}{\phi(\frac{\mathbf{x}+\mathbf{M}t/\varepsilon}{\varepsilon})} u(t,\mathbf{x} + \frac{\mathbf{M}t}{\varepsilon}) \sim U(t,\mathbf{x}) \tag{3.35}$$

3.1.4 Boundary conditions, boundary layers and the projection method

Does the multiple scale method extend to problems like (3.3, 3.4) over a bounded region $\mathcal{O}$ with given boundary conditions? We can also ask if the multiple scale method can be carried to higher order. Both questions depend on what one actually wants and, as is usual with asymptotic methods in general, it is much more important to know the widest conditions under which the principal term of the expansion is a valid approximation than to look for special situations where more accurate representations can be obtained. For initial value problems with rapidly oscillating periodic coefficients it is routine to carry the expansion to higher order provided that an appropriate initial layer expansion is constructed as well. As we will see in section 4 this is not possible for general stationary random coefficients. It is also not possible for problems in bounded domains except in a limited way as we now explain.

To illustrate the ideas let us consider a steady diffusion problem in a bounded domain

$$-\nabla \cdot \left(D(\frac{\mathbf{x}}{\varepsilon}) \nabla u(\mathbf{x}) \right) = f(\mathbf{x}) \tag{3.36}$$

with $x \in \mathcal{O}$ and $u(\mathbf{x}) = 0$ on the boundary $\partial\mathcal{O}$. For simplicity there is no reaction or convection so that $\phi = \psi = 1$ in (3.13, 3.14) and $\boldsymbol{\chi}(\mathbf{y}) = (\chi_j(\mathbf{y}))$ of (3.18) satisfies

$$\sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left(D(\mathbf{y})(\frac{\partial \chi_j}{\partial x_k} + \delta_{jk}) \right) = 0 \tag{3.37}$$

for $j = 1, 2, 3$ with χ_j unit periodic in each direction and with mean zero. The effective drift $\mathbf{M}$ is now zero and so is the effective reaction rate λ so that equation (3.19) becomes

$$-\sum_{i,j=1}^{3} D^*_{ij} \frac{\partial^2 \overline{u}}{\partial x_i \partial x_j} = f(\mathbf{x}) \tag{3.38}$$

with $\overline{u} = 0$ on $\partial\mathcal{O}$ and where instead of (3.23) we have

$$D^*_{ij} = \int_0^1 \int_0^1 \int_0^1 D(\mathbf{y}) \sum_{k=1}^{3} \left(\delta_{ik} + \frac{\partial \chi_i(\mathbf{y})}{\partial y_k} \right) \left(\delta_{jk} + \frac{\partial \chi_j(\mathbf{y})}{\partial y_k} \right) d\mathbf{y} \tag{3.39}$$

The solution u of (3.36) is approximated by $\overline{u}$ in the sense that from the multiple scale expansion we have

$$u(\mathbf{x}) = \overline{u}(\mathbf{x}) + \sum_{j=1}^{3} \varepsilon \chi_j(\frac{\mathbf{x}}{\varepsilon}) \frac{\partial \overline{u}(\mathbf{x})}{\partial x_j} + O(\varepsilon^2) \tag{3.40}$$

formally. In fact, using the maximum principle we see that we only have that $\max_{\mathbf{x}} |u(\mathbf{x}) - \overline{u}(\mathbf{x})| = O(\varepsilon)$ because the second term in the expansion (3.40) does not satisfy the boundary conditions and so we cannot do better.

Let $m^\varepsilon(\mathbf{x})$ be a cutoff function near $\partial\mathcal{O}$. This means that $m^\varepsilon(\mathbf{x})$ is a smooth function for $\varepsilon > 0$ that equals one except for an ε neighborhood of $\partial\mathcal{O}$ where it vanishes and in another ε neighborhood where it changes from one to zero in a smooth way. It is easy to see that if

$$z(\mathbf{x}) = u(\mathbf{x}) - \overline{u}(\mathbf{x}) - \sum_{j=1}^{3} \varepsilon \chi_j(\frac{\mathbf{x}}{\varepsilon}) \frac{\partial \overline{u}(\mathbf{x})}{\partial x_j} m^{\varepsilon}(\mathbf{x}) \tag{3.41}$$

then

$$\int_{\mathcal{O}} \left(z^2(\mathbf{x}) + |\nabla z(\mathbf{x})|^2 \right) d\mathbf{x} \leq C\varepsilon \tag{3.42}$$

where C is a constant independent of ε.

We may think of $m^{\varepsilon}(\mathbf{x})$ as a boundary layer correction to the expansion (3.40) except that it is an arbitrary cutoff function. The only information it contains about the problem is the width of the cutoff region near the boundary, which is of order ε. Is it possible to construct boundary layer corrections that reflect better the behavior of the solution near the boundary? This is a very difficult question even for problems with periodic structure, the case we are considering here, because the way a general boundary intercepts this structure can be very complicated. If the boundary is such that the local half-space problem obtained by stretching coordinates near some boundary point is a periodic one then boundary layer corrections can be constructed [28, 5]. Otherwise it does not seem possible to have the usual boundary layer behavior where boundary effects decay exponentially away from the boundary with a rate that is characteristic of the local medium-boundary structure.

One alternative is to replace the multiscale expansion with a *multiscale projection* [29] which we now describe briefly.

The boundary value problem (3.36) is the Euler equation of the quadratic functional

$$I^{\varepsilon}(w) = \frac{1}{2} \int_{\mathcal{O}} D(\frac{\mathbf{x}}{\varepsilon}) |\nabla w(\mathbf{x})|^2 d\mathbf{x} - \int_{\mathcal{O}} f(\mathbf{x}) w(\mathbf{x}) d\mathbf{x} \tag{3.43}$$

and the solution u is the minimizer of this functional. Motivated by the expansion (3.40) we try to minimize (3.43) over functions of the form

$$w(\mathbf{x}) = \overline{u}(\mathbf{x}) + \sum_{j=1}^{3} \varepsilon \chi_j(\frac{\mathbf{x}}{\varepsilon}) \overline{v}_j(\mathbf{x}) \tag{3.44}$$

with $\overline{u}$ and $\overline{v}_j$ are now the test functions that vanish on $\mathcal{O}$. We insert (3.44) into (3.43) and average over the rapidly oscillating terms while $\overline{u}$ and $\overline{v}_j$ are fixed. We get this way a new quadratic functional for $\overline{u}$ and $\overline{v}_j$. The Euler equations for this functional have the form

$$-\overline{D}\Delta\overline{u} - \sum_{j=1}^{3} \varepsilon\overline{D\chi_j}\Delta\overline{v}_j - \sum_{j=1}^{3} \overline{D\nabla\chi_j} \cdot \nabla\overline{v}_j = f \tag{3.45}$$

$$-\varepsilon\overline{D\chi_k}\Delta\overline{u} - \varepsilon^2 \sum_{j=1}^{3} \overline{D\chi_k\chi_j}\Delta\overline{v}_j + \overline{D\nabla\chi_k} \cdot \nabla\overline{u}$$

$$+\sum_{j=1}^{3} \overline{D\nabla\chi_k \cdot \nabla\chi_j}\overline{v}_j + \varepsilon\overline{D(\chi_j\nabla\chi_k - \chi_k\nabla\chi_j)} \cdot \nabla\overline{v}_j = 0 \quad, k = 1, 2, 3, \tag{3.46}$$

where the overline indicates average over the period cell. This is an elliptic system of equations for $\overline{u}$ and $\overline{v}_j$, $j = 1, 2, 3$, with $\overline{u}(\mathbf{x}) = 0$ and $\overline{v}_j(\mathbf{x}) = 0$, $j = 1, 2, 3$, on the boundary $\partial\mathcal{O}$. It has constant coefficients but it also depends explicitly on ε. If the cell functions $\chi_j(\mathbf{y})$ satisfy some simple nondegeneracy conditions [29] the system is nondegenerate elliptic and it is easy to see that as ε goes to zero $\overline{v}_j(\mathbf{x}) \to \frac{\partial\overline{u}(\mathbf{x})}{\partial x_j}$ and that the first equation in (3.45) becomes the same as (3.38). To verify this we need the identity $\overline{D\nabla\chi_p \cdot \nabla\chi_j} + \overline{D\nabla\chi_p}\delta_{pj} = 0$, $p, j = 1, 2, 3$, which follows from (3.37) after multiplying by χ_p, averaging over the cell and integrating by parts.

Of course, this behavior of (3.45) will be valid away from the boundary. The point of the multiscale projection method is that the asymptotic behavior of the homogenized elliptic system (3.45) on the one hand has the correct behavior in the interior and on the other it captures in an intrinsic way the boundary layer behavior of the original problem.

3.2 Random cell problem

Consider a conducting material occupying some region $\mathcal{D}$ in space and having conductivity equal to D_1 except inside spherical inclusions which have conductivity D_2. let $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$ denote the centers of the spherical inclusions and δ their radius. The conductivity $D(\mathbf{x})$ of the composite conductor is defined by

$$D(\mathbf{x}) = D(\mathbf{x}, \{\mathbf{y}_j\}, \delta) = \begin{cases} D_1 \ , \ |\mathbf{x} - \mathbf{y}_j| > \delta & \text{for all } j \ , \\ D_2 \ , \ |\mathbf{x} - \mathbf{y}_j| \le \delta & \text{for some } j \ . \end{cases} \tag{3.47}$$

Let $u(\mathbf{x}) = u(\mathbf{x}, \{\mathbf{y}_j\}, \delta)$ denote the temperature distribution is the conductor. Then u satisfies the equation

$$\nabla \cdot (D(\mathbf{x}) \nabla u(\mathbf{x})) = 0 \quad \text{on} \quad \mathcal{D} \tag{3.48}$$

with suitable boundary conditions on the boundary of $\mathcal{D}$.

When δ is small and the number N of spherical inclusions is large so that the occupied volume $\frac{4}{3}\pi\delta^3 N$ is of order one, the solution of (3.48) is a very difficult problem. One excepts however to be able to approximate $u(\mathbf{x})$ by two relatively simpler problems: one with constant or slowly changing coefficients over $\mathcal{D}$, the effective equation, and one that does not depend on the region $\mathcal{D}$ and depends only on the configuration $\{\mathbf{y}_j\}$ of the inclusions. The second problem, the *cell problem*, serves to define the effective conductivity that is used as a coefficient in the effective equation. The question of how the solution of an equation like (3.47) can be approximated by an effective equation is taken up in Chapter 4 in detail for the random case. We concentrate on the second problem here.

How should an effective conductivity be defined in the random case where we do not have a period cell? For such a concept to make sense it is necessary that the properties of the configuration $\{\mathbf{y}_j\}$ of inclusions depend only on their location relative to each other (for conceptual simplicity we do not consider somewhat more general configurations that still allow the definition of an effective conductivity). This means that the configuration must be infinite and translation invariant in a statistical sense, the generalization of periodicity. The inclusion centers in $\mathcal{D}$ must be a subset of such an infinite configuration $\{\mathbf{y}_j\}$ which we denote by ω.

Assume that we have an ensemble of configurations $\omega = \{\mathbf{y}_j\}$ whose statistical properties are translation invariant or stationary. Let $D(\mathbf{x}) = D(\mathbf{x}, \omega)$ denote the conductivity (3.47) which is now a stationary random function. Consider the following idealized, infinite medium problem. Find two vector fields $\mathbf{F}(\mathbf{x}, \omega)$ and $\mathbf{G}(\mathbf{x}, \omega)$, depending on the configuration ω, such that

$$\mathbf{F}(\mathbf{x}, \omega) = D(\mathbf{x}, \omega)\, \mathbf{G}(\mathbf{x}, \omega) \ , \tag{3.49}$$

$$\nabla \times \mathbf{G} = 0 \ , \tag{3.50}$$

$$\nabla \cdot \mathbf{F} = 0 \ , \tag{3.51}$$

$$\langle \mathbf{G} \rangle = \mathbf{e} \ . \tag{3.52}$$

In (3.52) $\langle\ \rangle$ denotes expectation or ensemble average over configurations ω with respect to the probability law over the ensemble and $\mathbf{e}$ stands for a fixed unit vector in space.

The solutions $\mathbf{F}(\mathbf{x},\omega)$ and $\mathbf{G}(\mathbf{x},\omega)$ are sought among vector fields that are stationary or translation invariant. As a result $\langle \mathbf{G} \rangle$ in (3.52) is a constant vector.

In the periodic case ω is a point in the period cell and $D(\mathbf{x},\omega)$ is equal to $D(\mathbf{x}+\omega)$ so that ω is just translation. The periodic cell problem, (3.37) for example, can be written in the form (3.49-3.52) by noting that $\mathbf{G} = \nabla\chi + \mathbf{e}$ and that the equation $\nabla \cdot (D(\nabla\chi + \mathbf{e})) = 0$ is (3.51).

The physical meaning of (3.49)–(3.52) is as follows. $\mathbf{F}$ is a heat flux vector and $-\mathbf{G}$ the negative temperature gradient. Equation (3.49) is Fourier's law of heat conduction. Equation(3.50) says that $\mathbf{G}$ is a gradient field locally and (3.51) that there are no sources or sinks. Equation (3.52) says that the average temperature gradient is in the direction $-\mathbf{e}$. If $\boldsymbol{\ell}$ is another unit vector, let

$$D^*(\mathbf{e},\boldsymbol{\ell}) = \langle \mathbf{F} \cdot \boldsymbol{\ell} \rangle \tag{3.53}$$

be the average heat flux in the direction $\boldsymbol{\ell}$ due to unit average temperature gradient in the direction $-\mathbf{e}$. It is a second order, symmetric, positive, tensor, by stationarity and because it depends linearly on $\mathbf{e}$ and $\boldsymbol{\ell}$. It is natural that D^* be called the effective conductivity. The symmetry and positive definiteness can be seen from the equivalent definition:

$$D^*(\mathbf{e},\boldsymbol{\ell}) = \langle D\,\mathbf{G}_e \cdot \mathbf{G}_\ell \rangle \ . \tag{3.54}$$

The equivalence of (3.53) and (3.54) follows in trum from the fact that $\mathbf{G}_\ell = \boldsymbol{\ell} + \widetilde{\mathbf{G}}_\ell$ with $\langle \widetilde{\mathbf{G}}_\ell \rangle = 0$ and $\nabla \times \widetilde{\mathbf{G}}_e = 0$ so that $\widetilde{\mathbf{G}}_\ell$ is a gradient. The rest is an integration by parts and (3.51). We do not go into the detailed verification of these steps here because they are taken up in the more general discussion in Chapter 4.

That (3.49)–(3.52) has a unique solution in a suitable weak sense is also taken up in Chapter 4. We analyze there the limiting behavior of the solution u of (3.48) as $N \to \infty$, $\delta \to 0$ so that $\frac{4}{3}\pi\delta^3 N \sim 1$ and show that u behaves like $\overline{u}$, the solution of $\nabla \cdot (D^*\,\nabla\overline{u}) = 0$ in $\mathcal{D}$ with suitable boundary conditions. This is a result of considerable interest that can be obtained in some generality. It establishes the existence of an effective description in a well defined macroscopic limit and identifies the effective coefficients via (3.49)–(3.53) which is a problem independent of the region $\mathcal{D}$ over which (3.48) is to be solved.

Once such general results become available, interest naturally shifts to the question: can we compute D^*? This question has had a history of over one hundred years and the answer is very much a research problem today. Even for periodic configurations of spherical inclusions, it is clear that D^* cannot be calculated exactly in more than one dimension.

3.3 The Maxwell-Claussius-Mossotti formula

To gain some perspective on what has been attempted, let us consider Maxwell's [12], 1873 analysis of the effective tensor. Let us assume that the distribution of inclusion centers is isotropic so that D^* is a scalar multiple of the identity.

Consider first the heat distribution outside a single sphere at the origin with radius δ. Let the temperature at infinity behave like $-\mathbf{x}\cdot\mathbf{e}$ with $\mathbf{e}$ a fixed unit vector. If we look for a solution of the form

$$\begin{aligned} &u = -\mathbf{x}\cdot\mathbf{e} + \chi(\mathbf{x}) \ , \qquad \chi = -A\frac{\mathbf{x}\cdot\mathbf{e}}{|\mathbf{x}|^3} \ , \qquad |\mathbf{x}| > \delta \ , \\ &u = -B\mathbf{x}\cdot\mathbf{e} \ , \qquad\qquad\quad |\mathbf{x}| < \delta \ , \end{aligned} \tag{3.55}$$

we find that

$$A = \delta^3\frac{D_1 - D_2}{2D_1 + D_2} \ , \quad B = \frac{3D_1}{2D_1 + D_2} \ . \tag{3.56}$$

Maxwell's argument is as follows. Suppose N spheres of radius δ are contained in a large sphere of radius R. Suppose that the spherical conductors outside this large sphere are ignored. If the relative volume $\beta = N\delta^3/R^3$ occupied by the inclusions is small then the temperature far away should be approximately equal to

$$-\mathbf{x}\cdot\mathbf{e}\left(1 + N\frac{\delta^3}{|\mathbf{x}|^3}\,\frac{D_1 - D_2}{2D_1 + D_2}\right) \ . \tag{3.57}$$

If the conducting material inside the sphere of radius R has effective conductivity D^*, the temperature far away should be

$$-\mathbf{x}\cdot\mathbf{e}\left(1 + \frac{R^3}{|\mathbf{x}|^3}\,\frac{D_1 - D^*}{2D_1 + D_2}\right) \ . \tag{3.58}$$

These expressions must be equal and hence

$$\frac{D^* - D_1}{D^* + 2D_1} = \beta\frac{D_2 - D_1}{D_2 + 2D_1} \ . \tag{3.59}$$

This is the famous Maxwell-Claussius-Mossotti formula which is supposed to be valid for $\beta \ll 1$ [13].

Through Maxwell's argument we have apparently solved (3.49)–(3.52) when the volume fraction β occupied by the inclusions is small and the sphere centers are isotropically distributed, in addition to being stationary. The result is (3.59) for the effective conductivity D^*.

3.4 The Rayleigh-Hasimoto method for a periodic distribution of inclusions

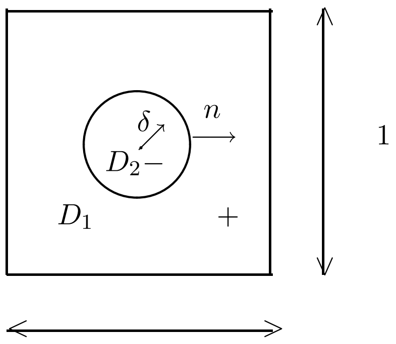
It is not easy to see why Maxwell's argument is correct and many attempts have been made to improve both the arguments and the results. The crucial point here is the way the geometric configuration of the inclusions affects D^*. Obviously then one should solve (3.49)–(3.52) in the periodic case since this should be the least involved. This was first done by Rayleigh [14], 1892, who notes in the beginning of this paper that he is not very comfortable with Maxwell's argument. He obtained the result

$$D^* = D_1 \left\{ 1 - \frac{3\beta}{\frac{2D_1+D_2}{D_1-D_2} + \beta - \frac{\alpha(D_1-D_2)}{\frac{4}{3}D_1+D_2}\beta^{10/3} + O(\beta^{14/3})} \right\} , \tag{3.60}$$

in which α is a constant eventually calculated to be 0.523 [15].

Note that (3.60) indeed agrees with (3.59) if only terms to order β are kept in the denominator in (3.60). More recently, Zuzovsky and Brenner [15] extended the analysis to $O(\beta^6)$ and it is possible to construct an asymptotic expansion for D^* to arbitrary order in β for β small. There is an elegant method for doing this which was first used for problems of the present form by Hasimoto [16]. This method has been implemented numerically yielding results that are valid for fairly large β [17]. We shall now use Hasimot's method to derive part of (3.60).

In a unit period cell (see figure) in $\mathbf{R}^3$



we must solve

$$\nabla \cdot (D(\mathbf{x})\, \nabla u) = 0 \ , \qquad\qquad (3.61)$$
$$u(\mathbf{x}) = x_1 + \chi(\mathbf{x}) \ , \quad \mathbf{x} = (x_1, x_2, x_3) \ , \quad \chi(\mathbf{x}) \text{ periodic,}$$

and then calculate

$$D^* = \langle D(1 + \frac{\partial \chi}{\partial x_1}) \rangle \ . \qquad (3.62)$$

Here $\langle \ \rangle$ denotes integration over a unit period cell and $D(\mathbf{x})$ equals D_1 outside the sphere of radius δ and D_2 inside. Note that (3.61) contains all of (3.49)–(3.52) the vector field $\mathbf{G}$ minus its mean will be derivable from a potential because of (3.50). But this potential will not be stationary in general. In the periodic case, stationarity is replaced by periodicity and any periodic, mean zero, curl-free vector field is derivable from a periodic potential.

Before analyzing (3.61) we note that as in Section 3.1 we have also the following two alternative expressions for D^*

$$D^* = \langle D \left(1 + \frac{\partial \chi}{\partial x_1}\right) \left(1 + \frac{\partial \chi}{\partial x_1}\right) \rangle \ , \qquad (3.63)$$

and

$$D^* = \int_{x_1 = s} D(\mathbf{x}) \left(1 + \frac{\partial \chi(\mathbf{x})}{\partial x_1}\right) dx_2\, dx_3 \ , \qquad (3.64)$$

where s is any number in $[-1/2, 1/2]$ and D^* of course does not depend on s. Both (3.63) and (3.64) follow easily from (3.61) and the divergence theorem (integration by parts).

How do we construct an expansion for D^* for δ small? Note first that (3.61) is equivalent to finding a periodic function $\chi(\mathbf{x})$ such that

$$\Delta \chi(\mathbf{x}) = 0 \quad \text{except on} \quad |\mathbf{x}| = \delta \ . \qquad (3.65)$$

$$\chi(\mathbf{x}) \quad \text{continuous across} \quad |\mathbf{x}| = \delta \ , \qquad (3.66)$$

$$D_1 \left(n_1 + \frac{\partial \chi}{\partial n}\right)_+ = D_2 \left(n_1 + \frac{\partial \chi}{\partial n}\right)_- \quad \text{on} \quad |\mathbf{x}| = \delta \ . \qquad (3.67)$$

here n_ℓ is the component in the x_ℓ-direction of the unit normal bfn, $\partial\chi/\partial n = \nabla\chi \cdot \mathbf{n}$ and plus–minus subscripts denote limiting values from outside and inside the sphere $|\mathbf{x}| = \delta$, respectively.

Let $G(\mathbf{x}, \mathbf{y})$ denote the unit periodic Green's function defined by

$$-\Delta_x\, G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) - 1 \ , \quad G \text{ periodic in } \mathbf{x}, \mathbf{y} \ , \qquad (3.68)$$

and normalized to have mean zero. Evidently

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^2} \sum_{\mathbf{m}\in\mathbf{Z}^3}{}' \frac{e^{2\pi i\mathbf{m}\cdot(\mathbf{x}-\mathbf{y})}}{|\mathbf{m}|^2} , \tag{3.69}$$

where the sum extends over all integer valued vectors with the prime denoting that the term with $\mathbf{m} = \mathbf{0}$ is omitted. The sum is conditionally convergent and we have

$$G(\mathbf{x},\mathbf{y}) \sim \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \quad \text{as} \quad |\mathbf{x}-\mathbf{y}| \to 0 . \tag{3.70}$$

This is to be expected since the effect of the periodic boundary conditions is negligible when source and observation point are very near each other. The expression (3.69) for G is called a *lattice sum* and its asymptotic behavior for $|\mathbf{x}-\mathbf{y}| \to 0$ has been studied extensively in many contexts in solid state physics [18].

We write $\chi(\mathbf{x})$ in the form

$$\chi(\mathbf{x}) = \int_{|\mathbf{y}|=\delta} G(\mathbf{x},\mathbf{y})\,\sigma(\mathbf{y})\,dS(\mathbf{y}) , \tag{3.71}$$

where the surface distribution σ is to be determined so that

$$\int_{|\mathbf{y}|=\delta} \sigma(\mathbf{y})\,dS(\mathbf{y}) = 0 . \tag{3.72}$$

Note that the ansatz (3.71) along with (3.72) satisfies (3.65) and (3.64) and that χ is indeed periodic. The continuity follows from (3.70) and the fact that the single layer potential

$$U(\mathbf{x}) = \int_{|\mathbf{y}|=\delta} \frac{\sigma(\mathbf{y})}{4\pi|\mathbf{x}-\mathbf{y}|}\,dS$$

is continuous across $|\mathbf{x}| = \delta$. We are looking for smooth σ in (3.71). From potential theory [19] we know that

$$\begin{aligned}
\left(\frac{\partial U}{\partial n}\right)_+ &= -\frac{\sigma}{2} + \int_{|\mathbf{y}|=\delta} \frac{\partial}{\partial n}\left(\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\right)\sigma(\mathbf{y})\,dS(\mathbf{y}) , \\
\left(\frac{\partial U}{\partial n}\right)_- &= \frac{\sigma}{2} + \int_{|\mathbf{y}|=\delta} \frac{\partial}{\partial n}\left(\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\right)\sigma(\mathbf{y})\,dS(\mathbf{y}) .
\end{aligned} \tag{3.73}$$

Note that the kernels in the integrals on the right are singular but with integrable singularity. Using (3.73), we can derive an integral equation for σ from (3.67)

$$D_1\left[-\frac{\sigma}{2}\int_{|\mathbf{y}|=\delta} \frac{\partial}{\partial n_x} G\,\sigma\,dS\right] - D_2\left[\frac{\sigma}{2} + \int_{|\mathbf{y}|=\delta} \frac{\partial}{\partial n_x} G\,\sigma\,dS\right] = (D_2 - D_1)n_1 .$$

where n_x denotes derivative with respect to $\mathbf{x}$ in the normal direction. This can be rearranged to become

$$\int_{|\mathbf{y}|=\delta} \frac{\partial}{\partial n_x} G(\mathbf{x},\mathbf{y})\,\sigma(\mathbf{y})\,dS(\mathbf{y}) + \frac{D_2+D_1}{D_2-D_1}\,\frac{\sigma(\mathbf{x})}{2} = -n_1(\mathbf{x}) \ , \qquad |\mathbf{x}| = \delta \tag{3.74}$$

which is the integral equation for σ. Note that (3.72) must hold and that the equation (3.64) is compatible with this.

Let

$$\mathbf{x} = \delta\boldsymbol{\xi} \ , \qquad \mathbf{y} = \delta\boldsymbol{\zeta} \ , \tag{3.75}$$

and define

$$\sigma^\delta(\boldsymbol{\zeta}) = \sigma(\delta\boldsymbol{\zeta}) \ , \quad G^\delta(\boldsymbol{\xi},\boldsymbol{\zeta}) = \delta G(\delta\boldsymbol{\xi},\delta\boldsymbol{\zeta}) \ . \tag{3.76}$$

We may write (3.74) in terms of these scaled quantities as follows:

$$\int_{|\boldsymbol{\zeta}|=1} \frac{\partial}{\partial n_\xi} G^\delta(\boldsymbol{\xi},\boldsymbol{\zeta})\,\sigma^\delta(\boldsymbol{\zeta})\,dS + \frac{D_2+D_1}{D_2-D_1}\,\frac{\sigma^\delta(\boldsymbol{\zeta})}{2} = -n_1(\boldsymbol{\xi}) \ , \quad |\boldsymbol{\xi}| = 1 \ . \tag{3.77}$$

The form (3.77) is suitable for an asymptotic expansion of σ^δ in powers of δ if the expansion of G^δ is known. Let us use just (3.70) to get the first term. We have that:

$$G^\delta(\boldsymbol{\xi},\boldsymbol{\zeta}) \to \frac{1}{4\pi|\boldsymbol{\xi}-\boldsymbol{\zeta}|} \ , \tag{3.78}$$

and

$$\sigma^\delta(\boldsymbol{\zeta}) \to \sigma^{(0)}(\boldsymbol{\zeta}) \quad \text{as} \quad \delta \to 0 \ . \tag{3.79}$$

It is verified easily either directly from (3.74) or from (3.71) and the jump conditions (3.73) that

$$\sigma^{(0)}(\boldsymbol{\zeta}) = 3\frac{D_1-D_2}{2D_1+D_2}\,n_1(\boldsymbol{\zeta}) \ . \tag{3.80}$$

Returning to (3.71) we see that for δ small

$$\begin{aligned} \chi(\mathbf{x}) &\sim 3\frac{D_1-D_2}{2D_1+D_2}\int_{|\mathbf{y}|=\delta} G(\mathbf{x},\mathbf{y})\,n_1(\mathbf{y})\,dS(\mathbf{y}) \ , \quad |\mathbf{x}| > \delta \\ &= 3\delta^2\frac{D_1-D_2}{2D_1+D_2}\int_{|\mathbf{y}|=1} G(\mathbf{x},\mathbf{y})\,n_1(\mathbf{y})\,dS(\mathbf{y}) \\ &\sim 4\pi\delta^3\frac{D_1-D_2}{2D_1+D_2}\,\frac{\partial}{\partial y_1}\,G(\mathbf{x},\mathbf{0}) \ . \end{aligned} \tag{3.81}$$

Here we use the fact that the integral of the normal over the sphere vanishes and that

$$\int_{|\mathbf{y}|=1} n_i(\mathbf{y})\,n_j(\mathbf{y})\,dS = \frac{1}{3}\delta_{ij} \ , \qquad i,j = 1,2,3 \ .$$

To evaluate D^* it is most convenient to use (3.64) with some $s \neq 0$. Then using (3.81) we have

$$D^* \sim D_1 \left[1 + 3\beta \frac{D_1 - D_2}{2D_1 + D_2} \int_{x_1 = s} \frac{\partial}{\partial x_1} \frac{\partial}{\partial y_1} G(\mathbf{x}, \mathbf{0}) \, dx_2 \, dx_3 \right] \ . \tag{3.82}$$

Now $\dfrac{\partial}{\partial y_1} G(\mathbf{x}, \mathbf{y}) = -\dfrac{\partial}{\partial x_1} G(\mathbf{x}, \mathbf{y})$ and because of (3.69) and the periodicity of G we have

$$- \int_{x_1 = S} \frac{\partial^2}{\partial x_1^2} G(\mathbf{x}, \mathbf{0}) \, dx_2 \, dx_3 = -1 \ ,$$

so that (3.82) gives

$$D^* = D_1 \left(1 - 3\beta \frac{D_1 - D_2}{2D_1 + D_2} + \cdots \right) \ , \qquad \beta \ll 1 \ , \tag{3.83}$$

which is the first term in (3.60).

It should be noted that (3.60) is not an expansion in powers (including fractional) of β since the denominator is not expanded. To obtain expansions of this form we should expand directly different functions of D^* (for example $(D^*)^{-1}$). Although the form of the expansion can play a big role in numerical accuracy, all these expansions will be asymptotically equivalent. The integral equation method is a convenient way to construct expansions to any order.

The construction of the expansion (3.83) depends of course on the ability to continue the expansion (3.70). This is a problem that is analyzed as follows [16]. We begin with the formula

$$\frac{1}{|\mathbf{m}|^2} = \pi \int_0^\infty e^{-\pi |\mathbf{m}|^2 \beta} \, d\beta \ . \tag{3.84}$$

Using (3.84) we write

$$\begin{aligned} \sum_{\mathbf{m}}{}' \frac{e^{2\pi i \mathbf{m} \cdot \mathbf{x}}}{|\mathbf{m}|^2} &= \pi \sum_{\mathbf{m}}{}' \int_0^\infty e^{-\pi |\mathbf{m}|^2 \beta + 2\pi i \mathbf{m} \cdot \mathbf{x}} \, d\beta \\ &= \pi \int_0^\infty \left(\sum_{\mathbf{m}} e^{-\pi \mathbf{m}^2 \beta + 2\pi i \mathbf{m} \cdot \mathbf{x}} - 1 \right) d\beta \ . \end{aligned} \tag{3.85}$$

Now we split the integral over β in (3.85) into two parts. One over $(0, \alpha)$ and one over (α, ∞) for some $\alpha > 0$. The sum is poorly convergent for β small, so in the range $0 \leq \beta \leq \alpha$ we transform it by the Poisson summation formula [20]

$$\sum_{\mathbf{m}} e^{-\pi \mathbf{m}^2 \beta + 2\pi i \mathbf{m} \cdot \mathbf{x}} = \frac{1}{\beta^{3/2}} \sum_{\mathbf{m}} e^{-\pi (\mathbf{x} - \mathbf{m})^2 / \beta} \ . \tag{3.86}$$

The sum on the right is also over all integer lattice points $\mathbf{m}$. The splitting depends on α, which must be chosen appropriately, but the expansion does not. The result is

$$G(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi|\mathbf{x} - \mathbf{y}|} - C + O\left(|\mathbf{x} - \mathbf{y}|^2\right) \ , \tag{3.87}$$

with C approximately equal to 2.8373 [16].

3.5 Conductivity in a medium with holes

The effective conductivity D^* of a composite material is defined quite generally by (3.49)–(3.53) provided $D(\mathbf{x}, \omega)$ is stationary and is bounded away from zero and infinity uniformly in $\mathbf{x}$ and ω, the configuration of the inclusions. In particular it is well defined for arbitrary volume fraction, although it can be usually calculated approximately for small volume fraction where interactions between inclusions are relatively weak. It should also be noted that the effective conductivity is the normalized average response to temperature gradients as can be seen from (3.53).

There are many problems for which the principal macroscopic effects appear at small volume fraction. In fact, in an asymptotic limit in which the volume fraction goes to zero. Wave propagation in bubbly fluids leads to such problems as well as many other situations in the study of multiple scattering. We will consider in this section what is perhaps the simplest example: heat removal in a conductor with many small holes. We will find that the effective heat removal rate is normalized response to temperature level, rather than temperature gradient. There are many other differences with the effective conductivity problem.

We formulate the problem as follows. Let $\mathbf{y}_1^N, \mathbf{y}_2^N, \ldots, \mathbf{y}_N^N$, $N = 1, 2, \ldots$, be a sequence of collections of points in $\mathbf{R}^3$ and consider a conducting medium of unit conductivity with spherical holes of radius δ centered about these points. Note that the hole centers $[\mathbf{y}_j^N]$ are a deterministic sequence of points at the moment and there are finitely many of them. Let $U^N(\mathbf{x}, t)$ be the temperature distribution in a region $\mathcal{D}$ containing the holes. Suppose the temperature is kept at zero (or some other fixed temperature) on the surface of the holes. Then U^N satisfies the equation

$$
\begin{aligned}
&U_t^N = \Delta U^N \ , && t > 0 \ , \qquad \mathbf{x} \text{ in } \mathcal{D} \text{ outside the holes,} \\
&U^N = 0 \ \text{ on the boundary of the holes} && \\
&U^N(0, \mathbf{x}) = f(\mathbf{x}) \ , &&
\end{aligned}
\tag{3.88}
$$

where $f(\mathbf{x})$ is the initial temperature distribution. We may give boundary conditions on $\partial\mathcal{D}$ but we concentrate on the problem of basic interest here which is the effect of the holes. So we assume $\mathcal{D} = \mathbf{R}^3$ but consider sets of points $[\mathbf{y}_j^N]$ that are all inside a compact set.

We want to find the behavior of U^N as the number of holes tends to infinity and the hole centers tend to a continuum. This means that if

$$
\Theta^N(A) = \frac{1}{N} \, \{\text{number of holes centers } \mathbf{y}_j^N \text{ in } A \subset \mathbf{R}^3\} \ , \tag{3.89}
$$

then,

$$
\Theta^N(A) \to \int_A \Theta(\mathbf{x}) \, d\mathbf{x} \quad \text{ as } \quad N \to \infty \tag{3.90}
$$

for all subsets A of $\mathbf{R}^3$. Here $\Theta(\mathbf{x})$ is the continuum hole center density, assumed to be a continuous nonnegative function with compact support. Of course as N tends to infinity the radius of holes δ must tend to zero so that at least the volume of the holes $N\delta^3$ is of order one.

There are many ways to analyze (3.88) [21], [22], [23], ranging from very analytical to very probabilistic, under a variety of assumptions on $[\mathbf{y}_j^N]$. We carry out a formal analysis by Green's functions to find out what the results are.

It is convenient to take Laplace transforms in (3.88) and replace U^N by

$$
\int_0^\infty e^{-\lambda t} \, U^N \, dt \ , \qquad \lambda > 0 \ .
$$

We denote again by U^N the transformed dependent variable which satisfies the equation

$$
(-\Delta + \lambda) U^N = f(\mathbf{x}) \ , \quad \mathbf{x} \text{ outside the holes} \tag{3.91}
$$

and the boundary conditions

$$
U^N(\mathbf{x}) = 0 \text{ for } |\mathbf{x} - \mathbf{y}_j^N| = \delta \ , \qquad j = 1, 2, \ldots, N \ , \quad \lambda > 0 \ . \tag{3.92}
$$

The initial temperature distribution $f(\mathbf{x})$ is assumed to be smooth and of compact support. Let $G_\lambda(\mathbf{x},\mathbf{y})$ be the Green's function

$$(-\Delta+\lambda)G_\lambda=\delta(\mathbf{x}-\mathbf{y})\ , \qquad \mathbf{x},\mathbf{y}\in \boldsymbol{R}^3 \tag{3.93}$$

which is given explicitly by

$$G_\lambda(\mathbf{x},\mathbf{y})=\frac{e^{-\sqrt{\lambda}|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}\ . \tag{3.94}$$

By Green's identity

$$\begin{aligned}&\textstyle\int_{\substack{\text{exterior}\\ \text{of the holes}}}\left[U^N(-\Delta+\lambda)G_\lambda-G_\lambda(-\Delta+\lambda)U^N\right]\,d\mathbf{y}\\ &=\textstyle\sum_{j=1}^N\int_{|\mathbf{y}-\mathbf{y}_j^N|=\delta}\left[U^N\frac{\partial G_\lambda}{\partial n}-G_\lambda\frac{\partial U^N}{\partial n}\right]\,dS\ .\end{aligned} \tag{3.95}$$

Here $\partial/\partial n$ denotes differentiation in the unit outward normal direction at the holes. Using (3.91) and (3.92), (3.95) becomes

$$U^N(\mathbf{x})=\int_{\text{exterior}}G_\lambda(\mathbf{x},\mathbf{y})\,f(\mathbf{y})\,d\mathbf{y}-\sum_{j=1}^N\int_{|\mathbf{y}-\mathbf{y}_j^N|=\delta}G_\lambda(\mathbf{x},\mathbf{y})\frac{\partial U^N(\mathbf{y})}{\partial n}\,dS(\mathbf{y})\ . \tag{3.96}$$

Suppose that as N tends to infinity and δ tends to zero in a suitable manner, $U^N(\mathbf{x})$ tends to a continuous limit $\overline{U}(\mathbf{x})$ which is smooth and everywhere defined. Let us look at what happens near a hole which we may assume is centered at the origin. When δ is very small and the other holes are far away, U^N satisfies approximately

$$\begin{aligned}&\Delta U^N=0\ ,\quad U^N=0\quad \text{on}\quad |\mathbf{x}|=\delta\\ &U^N\sim\overline{U}\quad \text{for}\quad |x|\gg\delta\ .\end{aligned} \tag{3.97}$$

In other words on the scale of the hole, temperature is a harmonic function (because λU^N and f are small compared to ΔU^N) with the value $\overline{U}$ away from its surface. Evidently the solution of (3.97) is $\overline{U}(1-\delta/|\mathbf{x}|)$. Assuming that the local temperature fields around each hole do not interact with each other, we may use this local form of U^N on the right side of (3.96). This gives

$$\sum_{j=1}^N\int_{|\mathbf{y}-\mathbf{y}_j^N|=\delta}G_\lambda(\mathbf{x},\mathbf{y})\frac{\partial U^N(\mathbf{y})}{\partial n}\,dS\sim\sum_{j=1}^N G_\lambda(\mathbf{x},\mathbf{y}_j^N)\,4\pi\,\delta^2\cdot\frac{\overline{U}(\mathbf{y}_j^N)}{\delta}\ . \tag{3.98}$$

Here we have used the limiting temperature $\overline{U}$ at $\mathbf{y}_j^N$ to set the temperature level for the local field around the j^{th} hole.

The continuum limit condition (3.90) is equivalent to assuming that for all continuous functions φ that vanish outside a bounded set

$$\frac{1}{N}\sum_{j=1}^{N}\varphi(\mathbf{y}_j^N) \to \int \varphi(y)\,\Theta(\mathbf{y})\,d\mathbf{y} \quad \text{as} \quad N\to\infty\ . \tag{3.99}$$

Now we look at the right side of (3.98) and note that in order to be able to apply (3.99), δ must be of order N^{-1}. This fixes the unknown up to now scaling

$$N\to\infty\ , \qquad \delta\to 0\ , \qquad N\delta = 1\ , \tag{3.100}$$

for the continuum limit. Using (3.99) in (3.98) and then the result in (3.96) we obtain the following integral equation for the continuum limit $\overline{U}$

$$\overline{U}(\mathbf{x}) = \int G_\lambda(\mathbf{x},\mathbf{y})\,f(\mathbf{y})\,d\mathbf{y} - \int G_\lambda(\mathbf{x},\mathbf{y})\,4\pi\,\Theta(\mathbf{y})\,\overline{U}(\mathbf{y})\,d\mathbf{y}\ . \tag{3.101}$$

This is equivalent to the equation

$$(-\Delta+\lambda)\overline{U} + 4\pi\,\Theta\,\overline{U} = f\ , \qquad \mathbf{x}\in\mathbf{R}^3\ . \tag{3.102}$$

After inverting the Laplace transform this becomes

$$\begin{cases} \overline{U}_t = \Delta\overline{U} - 4\pi\Theta\overline{U}\ , & t>0\ , \quad \mathbf{x}\in\mathbf{R}^3\ , \\ \overline{U}(0,\mathbf{x}) = f(\mathbf{x}) \end{cases} \tag{3.103}$$

We have found that in the continuum limit (3.100) the temperature U^N behaves like $\overline{U}$ which satisfies (3.103). In the continuum limit the effect of the holes is replaced by the local heat removal rate $4\pi\Theta\overline{U}$. The rate at which heat is removed by the holes around x is

$$\begin{aligned} \textstyle\sum_{j=1}^{N}\varphi(\mathbf{y}_j^N)\int_{|\mathbf{y}-\mathbf{y}_j^N|=\delta}\frac{\partial U^N}{\partial n}\,dS \quad &\sim 4\pi\delta\textstyle\sum_{j=1}^{N}\varphi(\mathbf{y}_j^N)\,\overline{U}(\mathbf{y}_j^N) \\ &\sim 4\pi\textstyle\int\varphi(\mathbf{y})\,\Theta(\mathbf{y})\,\overline{U}(\mathbf{y})\ , \end{aligned} \tag{3.104}$$

where $\varphi(\mathbf{y})$ is an arbitrary continuous function which is zero outside a small neighborhood of $\mathbf{x}$. So $4\pi\Theta\overline{U}$ is the rate at which heat is removed per hole ($\sim 4\pi\,\delta\,\overline{U}$) times the number of holes per unit volume $N\Theta$. Note that the pricipal macroscopic effects occur as the volume of the holes $\sim N\delta^3 = \delta^2$ goes to zero. If instead of (3.100) we have $N\to\infty$, $\delta\to 0$ with $N\delta\to 0$ then the limit satisfies

$$\begin{aligned} &\overline{U}_t = \Delta\overline{U}\ , \qquad && t>0\ , \quad \mathbf{x}\in\mathbf{R}^3\ , \\ &\overline{U}(0,\mathbf{x}) = f(\mathbf{x})\ , && \end{aligned}$$

and the effect of the holes disappears. There are not enough holes to have an effect. If on the other hand $N \to \infty$, $\delta \to 0$ and $N\delta \to \infty$ then the limit satisfies

$$\begin{aligned}
&\overline{U} = \Delta \overline{U} \ , \ t > 0 \ , \ \mathbf{x} \text{ outside the support of } \Theta \ , \\
&\overline{U}(0, \mathbf{x}) = f(\mathbf{x}) \ , \\
&\overline{U}(t, \mathbf{x}) = 0 \text{ on the boundary of the support of } \Theta \ .
\end{aligned}$$

This means that the holes behave in the limit as one big hole at the support of the continuum density Θ. It is in the limit (3.100) that a balance of effects is achieved.

Once it is realized that (3.100) is the correct asymptotic limit, the main burden of the analysis is in showing that the local fields around each hole, which are of the form const. $\delta|\mathbf{x} - \mathbf{y}_j^N|^{-1}$, do not interact with each other. At the k^{th} hole the effect of the local fields of the other holes is of the order of ($\delta = 1/N$)

$$\frac{1}{N} \sum_{\substack{j=1 \\ j \neq k}}^{N} \frac{1}{|\mathbf{y}_k^N - \mathbf{y}_j^N|} \ .$$

It is necessary to have some control on this expression and (3.90) or (3.99) are not enough. If for example

$$\max_{k=1,2,\ldots,N} \left| \frac{1}{N} \sum_{\substack{j=1 \\ j \neq k}}^{N} \frac{1}{|\mathbf{y}_k^N - \mathbf{y}_j^N|} - \int \frac{\Theta(\mathbf{y})}{|\mathbf{y}_k^N - \mathbf{y}|} \, d\mathbf{y} \right| \to 0 \quad \text{as} \quad N \to \infty \ , \tag{3.105}$$

then [21], [22], [23] the interaction can be controlled and shown to be negligible. Instead of (3.105) one may be tempted to take a simpler condition like

$$\min_{i \neq j} |\mathbf{y}_i^N - \mathbf{y}_j^N| \geq \gamma \, N^{-1/3} \ , \tag{3.106}$$

where γ is a constant independent of N. This simply says that the interhole distance never falls below a minimum which is a fixed fraction of the typical interhole distance $N^{-1/3}$. An assumption like (3.106) is undesirable because it is not true for a random distribution of points.

In fact, random distributions of points can be treated realization by realization [22] provided that conditions (3.90) and (3.105) hold. In the case $[\mathbf{y}_j^N]$ are independent random variables (3.90) holds with probability one since it is the strong law of large numbers. Condition (3.105) holds in probability in this case but one can show easily that

$$P\left[\min_{i \neq j} |\mathbf{y}_i^N - \mathbf{y}_j^N| \geq \delta N^{-1/3} \right] \to 0 \quad \text{as} \quad N \to \infty \ ,$$

for all $\gamma > 0$. Under condition (3.105) the random case can be treated realization by realization for those realizations for which (3.105) holds with prescribed accuracy. The set of such realizations has probability arbitrarily close to one and this leads to the desired results (see also [24], [25]).

Wave propagation in bubbly liquids can be analyzed by similar methods, in the regime of low volume fraction for the bubbles and propagation of long waves [26].

3.6 The Floquet-Bloch representation

3.6.1 Periodization

We will analyze convection-diffusion equations with periodic coefficients

$$\frac{\partial u}{\partial t} + \mathbf{v}(\mathbf{x}) \cdot \nabla u = \nabla \left(D(\mathbf{x}) \nabla u \right) \ . \tag{3.107}$$

The diffusivity $D(\mathbf{x})$ is positive and bounded and the convective velocity $\mathbf{v}(\mathbf{x})$ may or may not be divergence free but both are periodic with period 1 in each direction. The initial conditions are

$$u(0, \mathbf{x}) = f(\mathbf{x}) \tag{3.108}$$

and f is a smooth function of compact support (not periodic).

We will get an exact representation of the solution of (3.107) by exploiting the periodic structure of the coefficients, much as we do with the Fourier transform in the case of constant coefficients. The first step is *periodization*. Let

$$L(\mathbf{x}) = \nabla \cdot (D(\mathbf{x}) \nabla \cdot) - \mathbf{v}(\mathbf{x}) \cdot \nabla \tag{3.109}$$

and put

$$u(t, \mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} w(t, \mathbf{x}) \tag{3.110}$$

where $\mathbf{k}$ is a vector. The function w satisfies

$$\begin{aligned} w_t &= e^{-i\mathbf{k}\cdot\mathbf{x}} L(\mathbf{x}) \left(e^{i\mathbf{k}\cdot\mathbf{x}} w \right) \\ w(0, \mathbf{x}) &= e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) \end{aligned} \tag{3.111}$$

Define the "shifted" L operator by

$$L(\mathbf{k},\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} L(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \tag{3.112}$$

or more explicitly by

$$L(\mathbf{k},\mathbf{x}) = (i\mathbf{k}+\nabla)\cdot(D(\mathbf{x})(i\mathbf{k}+\nabla)\cdot) - \mathbf{v}(\mathbf{x})\cdot(ik+\nabla) \tag{3.113}$$

Then $w(t,\mathbf{x})$ satisfies

$$\begin{aligned} w_t &= L(\mathbf{k},\mathbf{x})w \\ w(0,\mathbf{x}) &= e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) \end{aligned} \tag{3.114}$$

Now let

$$\widetilde{w}(t,\mathbf{x}) = \sum_{\mathbf{m}} w(t,\mathbf{x}+\mathbf{m}) \tag{3.115}$$

where the sum is over all vectors $\mathbf{m}$ with integer coefficients ($\mathbf{m} = (m_1, m_2, m_3)$, $m_j = 0, \pm 1, \pm 2, \ldots,\ j = 1,2,3$). Clearly $\tilde{w}(t,\mathbf{x})$ is **periodic** in each direction with period one. Let similarly

$$\tilde{f}(\mathbf{x}) = \sum_{\mathbf{m}} e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{m})} f(\mathbf{x}+\mathbf{m}) \tag{3.116}$$

which is also periodic. Since the coefficients of $L(\mathbf{k},\mathbf{x})$ are periodic in $\mathbf{x}$ we have that

$$L(\mathbf{k},\mathbf{x}+\mathbf{m}) = L(\mathbf{k},\mathbf{x})$$

for all integer vectors $\mathbf{m}$. Thus

$$\begin{aligned} \widetilde{w}_t &= L(\mathbf{k},\mathbf{x})\widetilde{w} \\ \widetilde{w}(0,\mathbf{x}) &= \tilde{f}(\mathbf{x}) \end{aligned} \tag{3.117}$$

is a **periodic** problem in $\mathbf{x} = (x_1, x_2, x_3)$ with

$$0 \le x_j \le 1 \quad , \quad j = 1,2,3$$

for each vector $\mathbf{k} = (k_1, k_2, k_3)$ with

$$0 \le k_j \le 2\pi \quad , \quad j = 1,2,3\ .$$

Once problem (3.117) is solved and $\widetilde{w} = \widetilde{w}(t, \mathbf{x}; \mathbf{k})$ is determined, we can recover the solution $u(t, \mathbf{x})$ of the original problem (3.107), (3.108) as follows. From (3.115) and (3.110) we have

$$\widetilde{w}(t, \mathbf{x}; \mathbf{k}) = \sum_{\mathbf{m}} e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{m})} u(t, \mathbf{x}+\mathbf{m})$$

and hence

$$e^{i\mathbf{k}\cdot\mathbf{x}} \widetilde{w}(t, \mathbf{x}; \mathbf{k}) = \sum_{\mathbf{m}} e^{-i\mathbf{k}\cdot\mathbf{m}} u(t, \mathbf{x}+\mathbf{m}) \tag{3.118}$$

Integrating (3.118) over $\mathbf{k}$ in $[0, 2\pi]^3$ we get

$$u(t, \mathbf{x}) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}} \widetilde{w}(t, \mathbf{x}; \mathbf{k}) d\mathbf{k} \tag{3.119}$$

The main point of the above calculation is that a problem like (3.107), (3.108) that has periodic coefficients can be reduced exactly to the solution of a periodic initial value problem (3.117) and a quadrature (3.119). For numerical calculations this is an important reduction and, depending on the complexity of the periodic coefficients, can be a competitive method. We may call this method solution by *periodization*.

3.6.2 Spectral representation

We can use spectral theory to represent the solution of the periodic problem (3.117). The spectral theory will be for the family of elliptic operators $L(\mathbf{k}, \mathbf{x})$ on the unit period cell $\mathbf{x} \in [0, 1]^3$ for each $\mathbf{k} \in [0, 2\pi]^3$. The operator $L(\mathbf{k}, \mathbf{x})$ is **not** selfadjoint in general, when the flow field $\mathbf{v}(\mathbf{x})$ is not zero. However, it is an operator with compact resolvent and therefore we know that it has a complete set of eigenfunctions and discrete eigenvalues

$$\begin{aligned} L(\mathbf{k}, \mathbf{x})\phi_p(\mathbf{x}; \mathbf{k}) + \lambda_p(\mathbf{k})\phi_p(\mathbf{x}; \mathbf{k}) = 0 \\ p = 1, 2, \ldots, \quad \mathbf{k} \in [0, 2\pi]^3 \end{aligned} \tag{3.120}$$

with $\phi_p(\mathbf{x}; \mathbf{k})$ unit periodic in $\mathbf{x}$. The adjoint equation

$$L^\star(\mathbf{k}, \mathbf{x})\psi_p(\mathbf{x}, \mathbf{k}) + \overline{\lambda_p}(\mathbf{k})\psi_p(\mathbf{x}; k) = 0 \tag{3.121}$$

also has solutions and, in general, they are orthogonal with the eigenfunction ϕ_p

$$\int_0^1 \int_0^1 \int_0^1 \phi_p(\mathbf{x}; \mathbf{k}) \overline{\psi_q(\mathbf{x}; \mathbf{k})} d\mathbf{x} = \delta_{pq} \tag{3.122}$$

We can solve (3.117) by eigenfunction expansion.

$$\widetilde{w}(t,\mathbf{x};\mathbf{k}) = \sum_{p=1}^{\infty} e^{-\lambda_p(\mathbf{k})t} c_p \phi_p(\mathbf{x};\mathbf{k}) \tag{3.123}$$

with the constants c_p determined from the initial condition by the biorthogonality (3.122)

$$c_p(\mathbf{k}) = \int_0^1\int_0^1\int_0^1 \tilde{f}(\mathbf{x})\overline{\psi_p(\mathbf{x};\mathbf{k})}d\mathbf{x} \tag{3.124}$$

The solution $u(t,\mathbf{x})$ of (3.107), (3.108) can now be recovered from (3.119) and (3.123)

$$u(t,\mathbf{x}) = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{p=1}^{\infty} e^{-\lambda p(\mathbf{k})t} c_p(\mathbf{k})\phi_p(\mathbf{x};\mathbf{k})d\mathbf{k} \tag{3.125}$$

Letting $t=0$ in (3.125) we get the Floquet-Bloch decomposition of a function $f \in C_0^\infty$

$$f(\mathbf{x}) = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{p=1}^{\infty} c_p(\mathbf{k})\phi_p(\mathbf{x};\mathbf{k})d\mathbf{k} \tag{3.126}$$

with the coefficients $c_p(\mathbf{k})$ given by (3.124) and (3.116)

$$\begin{aligned} c_p(\mathbf{k}) &= \int_0^1\int_0^1\int_0^1 \sum_{\mathbf{m}} e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{m})} f(\mathbf{x}+\mathbf{m})\overline{\psi_p(\mathbf{x};k)}d\mathbf{x} \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\overline{\psi_p(\mathbf{x};\mathbf{k})}d\mathbf{x} \end{aligned} \tag{3.127}$$

where we have used the fact that $\psi(\mathbf{x};k)$ is unit periodic in $\mathbf{x}$ so that $\psi_p(\mathbf{x}+\mathbf{m};\mathbf{k}) = \psi_p(\mathbf{x};\mathbf{k})$.

The expansion of $f(\mathbf{x})$ can also be given with ψ_p, the adjoint eigenfunctions, as the primary ones. This is done by starting with the adjoint operator $L^\star$ rather than L in (3.109). We then get, instead of (3.126), (3.127),

$$f(\mathbf{x}) = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{p=1}^{\infty} d_p(\mathbf{k})\psi_p(\mathbf{x};\mathbf{k})d\mathbf{k} \tag{3.128}$$

with

$$d_p(\mathbf{k}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\overline{\phi_p(\mathbf{x};k)}d\mathbf{x} \tag{3.129}$$

From these two expansions we also get

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |f(\mathbf{x})|^2\, d\mathbf{x} = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} d\mathbf{k} \sum_{p=1}^{\infty} c_p(\mathbf{k})\overline{d_p(\mathbf{k})} \tag{3.130}$$

The most direct way to derive (3.130) is to start with the expansions of the periodized f in (3.116)

$$\tilde{f}(\mathbf{x}) = \sum_{p=1}^{\infty} c_p(\mathbf{k})\phi_p(\mathbf{x};\mathbf{k}) \tag{3.131}$$

$$\tilde{f}(\mathbf{x}) = \sum_{q=1}^{\infty} d_q(\mathbf{k})\psi_q(\mathbf{x};\mathbf{k}) \tag{3.132}$$

From the biorthogonality (3.122) we get

$$\int_0^1\int_0^1\int_0^1 \left|\tilde{f}(\mathbf{x})\right|^2 d\mathbf{x} = \sum_{p=1}^{\infty} c_p(\mathbf{k})d_p(\mathbf{k}) \tag{3.133}$$

Integrating both sides of (3.133) with respect to $\mathbf{k}$ and using (3.116) we get (3.130).

In the selfadjoint case, when for example there is no convection $\mathbf{v}(\mathbf{x}) \equiv 0$, (3.130) becomes Parseval's relation for the Floquet-Bloch expansion (3.126), (3.127)

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |f(\mathbf{x})|^2\, d\mathbf{x} = \frac{1}{(2\pi)^3}\int_0^{2\pi}\int_0^{2\pi}\int_0^{2\pi} d\mathbf{k}\sum_{p=1}^{\infty}|c_p(\mathbf{k})|^2 \tag{3.134}$$

The non-selfadjoint case is, in general, much more difficult to analyze and to give more precise meaning to the Floquet-Bloch expansion [30].

From the computational point of view, if one wants to solve (3.107) and (3.108), it is best to work directly with the periodized problem (3.117) and then recover the solution from (3.119). The spectral representation is a rather delicate object, certainly in the non-selfadjoint case, and should be used sparingly.

3.6.3 Homogenization from the Floquet-Bloch representation

How does homogenization fit into the picture we have from the Floquet-Bloch representation? We start with (3.107) but consider initial data of the form

$$u(0,\mathbf{x}) = f(\varepsilon\mathbf{x}) \tag{3.135}$$

where $\varepsilon > 0$ is a small parameter. We want to solve the convection diffusion equation for a long time when the initial concentration is slowly varying with respect to the periodic structure of the coefficients of (3.107). We change variables to long space and time units:

$\mathbf{x} \to \mathbf{x}/\varepsilon$ and $t \to t/\varepsilon^2$. Then we have the convection diffusion problem

$$\frac{\partial u}{\partial t} + \frac{1}{\varepsilon}\mathbf{v}\left(\frac{\mathbf{x}}{\varepsilon}\right) \cdot \nabla u = \nabla \cdot \left(D\left(\frac{\mathbf{x}}{\varepsilon}\right)\nabla u\right) \tag{3.136}$$

$$u(0,\mathbf{x}) = f(\mathbf{x}) \tag{3.137}$$

in macroscopic space-time units. As in section 3.1, we want to get the small ε behavior of the solution but now from the Floquet-Bloch representation, without a multiple scale expansion. This is primarily a pedagogical exercise because the small ε limit, homogenization, can be carried out directly much more efficiently and in much greater generality, as we saw in section 3.1 and we will see again in section 4. But it is a useful exercise because we can see explicitly how the asymptotic form of the solution develops from the exact one.

Since the period cell is now $[0,\varepsilon]^3$ the dual, or wavenumber, cell for $\mathbf{k}$ can be taken to be $[-\pi/\varepsilon, \pi/\varepsilon]^3$. Thus the solution of (3.136) is

$$u(t,\mathbf{x}) = \frac{1}{(2\pi)^3}\int_{-\pi/\varepsilon}^{\pi/\varepsilon}\int_{-\pi/\varepsilon}^{\pi/\varepsilon}\int_{-\pi/\varepsilon}^{\pi/\varepsilon} e^{i\mathbf{k}\cdot\mathbf{x}}\sum_{p=1}^{\infty} e^{-\lambda_p(\varepsilon\mathbf{k})t/\varepsilon^2}$$

$$\cdot\ \varepsilon^3 c_p(\mathbf{k})\phi_p\left(\frac{\mathbf{x}}{\varepsilon}, \varepsilon\mathbf{k}\right) d\mathbf{k} \tag{3.138}$$

$$\varepsilon^3 c_p(\mathbf{k}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\overline{\psi_p\left(\frac{\mathbf{x}}{\varepsilon}, \varepsilon\mathbf{k}\right)} d\mathbf{x} \tag{3.139}$$

where $\phi_p(\mathbf{x};\mathbf{k})$, $\psi_p(\mathbf{x},\mathbf{k})$ and $\lambda_p(\mathbf{k})$ satisfy (3.120) and (3.121) for the unit cell problem. It is clear from (3.138), (3.139) that we must analyze $\phi_p(\mathbf{x};\varepsilon\mathbf{k})$ and $\lambda_p(\varepsilon\mathbf{k})$ for ε small. We write the generator $L(\mathbf{x},\varepsilon\mathbf{k})$ in the form

$$L(\mathbf{x},\varepsilon\mathbf{k}) = L_0 + \varepsilon L_1 + \varepsilon^2 L_2 \tag{3.140}$$

with

$$L_0 = \nabla\cdot(D(\mathbf{x})\nabla) - \mathbf{v}(x)\cdot\nabla \tag{3.141}$$

$$L_1 = D(\mathbf{x})i\mathbf{k}\cdot\nabla + i\mathbf{k}\cdot\nabla(D(\mathbf{x})\cdot) - i\mathbf{k}\cdot\mathbf{v}(\mathbf{x}) \tag{3.142}$$

$$L_2 = -k^2 D(\mathbf{x}) \tag{3.143}$$

Expanding ϕ_p and λ_p

$$\phi_p(\mathbf{x},\varepsilon\mathbf{k}) = \phi_p^{(0)}(\mathbf{x}) + \varepsilon\phi_p^{(1)}(\mathbf{x}) + \ldots \tag{3.144}$$

$$\lambda_p(\varepsilon\mathbf{k}) = \lambda_p^{(0)} + \varepsilon\lambda_p^{(1)} + \varepsilon^2\lambda_p^{(2)} + \ldots \tag{3.145}$$

we get from (3.120) the following sequence of problems

$$L_0\phi_p^{(0)} + \lambda_p^{(0)}\phi_p^{(0)} = 0 \tag{3.146}$$

$$L_0\phi_p^{(1)} + \lambda_p^{(0)}\phi_p^{(1)} + L_1\phi_p^{(0)} + \lambda_p^{(1)}\phi_p^{(0)} = 0 \tag{3.147}$$

$$L_0\phi_p^{(2)} + \lambda_p^{(0)}\phi_p^{(2)} + L_1\phi_p^{(1)} + L_2\phi_p^{(0)} + \lambda_p^{(1)}\phi_p^{(1)} + \lambda_p^{(2)}\phi_p^{(0)} = 0 \tag{3.148}$$

From (3.141) and (3.146) we conclude that for $p = 1$, the principal eigenvalue, we have

$$\phi_1^{(0)} \equiv 1 \quad , \quad \lambda_1^{(0)} = 0 \tag{3.149}$$

We will only consider perturbations of this eigenvalue-eigenfunction. For the first correction we get from (3.147)

$$L_0\phi_1^{(1)} + L_1\phi_1^{(0)} + \lambda_1^{(0)} = 0 \ . \tag{3.150}$$

or more explicitly

$$\nabla \cdot (D\nabla\phi_1^{(1)}) - \mathbf{v} \cdot \nabla\phi_1^{(1)} + i\mathbf{k} \cdot \nabla D - i\mathbf{k} \cdot \mathbf{v} + \lambda_1^{(1)} = 0 \ . \tag{3.151}$$

The adjoint eigenfunction $\psi_1^{(0)}$ for (3.146) is not identically equal to 1 as in (3.149) unless the convective flow $\mathbf{v}(\mathbf{x})$ is incompressible ($\nabla \cdot \mathbf{v} = 0$). In general $\psi_1^{(0)}$ satisfies

$$\nabla \cdot \left(D\nabla\psi_1^{(0)}\right) + \nabla \cdot \left(\mathbf{v}\psi_1^{(0)}\right) = 0 \tag{3.152}$$

and is a positive, unit periodic function. We normalize it so that its integral over the unit cell is one.

We now multiply (3.151) with $\psi_1^{(0)}(\mathbf{x})$ and integrate over the unit cell. This determines $\lambda_1^{(1)}$

$$\lambda_1^{(1)} = ik \cdot \int_0^1\int_0^1\int_0^1 \left(\mathbf{v}(\mathbf{x}) - \nabla D(\mathbf{x})\right)\psi_1^{(0)}(\mathbf{x})d\mathbf{x} = i\mathbf{k} \cdot \mathbf{M} \tag{3.153}$$

and so $\phi_1^{(1)}$ satisfies (3.151) which is now solvable. We know that for the elliptic operator L_0 (defined by (3.141)) over the unit cell $\lambda_1^{(0)} = 0$ is an isolated eigenvalue so the Fredholm alternative holds for the inhomogeneous equation (3.151). Let $\boldsymbol{\chi}(\mathbf{x})$ be the solution of

$$\nabla \cdot (D\nabla\boldsymbol{\chi}) - \mathbf{v} \cdot \nabla\boldsymbol{\chi} - (\mathbf{v} - \nabla D - \mathbf{M}) = 0 \tag{3.154}$$

over the unit period cell, normalized to leave mean zero. Here $\mathbf{M}$ is the mean of $\mathbf{v} - \nabla D$ defined by (3.153). In terms of $\boldsymbol{\chi}$ we can write $\phi_1^{(1)}$ in the form

$$\phi_1^{(1)} = i\mathbf{k} \cdot \boldsymbol{\chi} \tag{3.155}$$

We consider now (3.148) which can be written more explicitly in the form

$$\begin{aligned}\nabla \cdot \left(D\nabla\phi_1^{(2)}\right) - \mathbf{v} \cdot \nabla\phi_1^{(2)} & \\ &+ \left(Di\mathbf{k} \cdot \nabla\phi_1^{(1)} + i\mathbf{k} \cdot \nabla(D\phi_1^{(1)}) - i\mathbf{k} \cdot \mathbf{v}\phi_1^{(1)}\right) \\ &- k^2 D + i\mathbf{k} \cdot \mathbf{M}\phi_1^{(1)} + \lambda_1^{(2)} = 0\ .\end{aligned} \tag{3.156}$$

The solvability condition for this equation determines $\lambda_1^{(2)}$ which, along with (3.155) and (3.153), gives

$$\begin{aligned}\lambda_1^{(2)} = \int_0^1 \int_0^1 \int_0^1 \Big[& k^2 D + 2D\mathbf{k} \cdot \nabla(\mathbf{k} \cdot \boldsymbol{\chi}) \\ &- \mathbf{k} \cdot (\mathbf{v} - \nabla D - \mathbf{M})\mathbf{k} \cdot \boldsymbol{\chi}\Big]\, \psi_1^{(0)} d\mathbf{x}\end{aligned} \tag{3.157}$$

We can express (3.157) in a form that displays its positivity as follows. We multiply (3.154) by $\psi_1^{(0)}\boldsymbol{\chi}$, integrate over the unit cell, integrate by parts and use (3.152). This gives the identity

$$\begin{aligned}-\int_0^1 \int_0^1 \int_0^1 \mathbf{k} \cdot (\mathbf{v} - \nabla D - \mathbf{M})\mathbf{k} \cdot \boldsymbol{\chi}\psi_1^{(0)} d\mathbf{x} & \\ &= \int_0^1 \int_0^1 \int_0^1 D\, (\nabla(\mathbf{k} \cdot \boldsymbol{\chi}))^2\, \psi_1^{(0)} d\mathbf{x}\end{aligned} \tag{3.158}$$

We can therefore write (3.157) in the form

$$\lambda_1^{(2)} = \sum_{i,j=1}^{3} k_i k_j D_{ij}^* \tag{3.159}$$

where

$$D_{ij}^* = \sum_{p=1}^{3} \int_0^1 \int_0^1 \int_0^1 D\psi_1^{(0)} \left(\delta_{ip} + \frac{\partial \chi_i}{\partial x_p}\right)\left(\delta_{jp} + \frac{\partial \chi_j}{\partial x_p}\right) d\mathbf{x} \tag{3.160}$$

which shows that D_{ij}^* is symmetric and $\lambda_1^{(2)}$ is positive definite as a quadratic form in $\mathbf{k}$.

Returning to (3.138), (3.139) and using the results of the expansion in powers of ε we get the small ε behavior of the solution u of (3.136), (3.137):

$$u(t, \mathbf{x}) \sim \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{M}t/\varepsilon - \mathbf{k}\mathbf{k}:\mathbf{D}^* t} \hat{f}(\mathbf{k}) d\mathbf{k} \tag{3.161}$$

where

$$\mathbf{k}\mathbf{k} : \mathbf{D}^* = \sum_{i,j=1}^{3} k_i k_j D_{ij}^* \tag{3.162}$$

and $\hat{f}(\mathbf{k})$ is the Fourier transform of $f(\mathbf{x})$. It is easy to see that if $\overline{u}(t,\mathbf{x})$ stands for the integral in (3.161) then it satisfies the constant coefficient diffusion equation

$$\frac{\partial \overline{u}}{\partial t} + \frac{1}{\varepsilon}\mathbf{M} \cdot \nabla \overline{u} = \nabla \cdot (D^* \nabla \overline{u}) \tag{3.163}$$

$$\overline{u}(0,\mathbf{x}) = f(\mathbf{x}) \tag{3.164}$$

The mean velocity is given by (3.153) and the effective diffusivity (a constant matrix) is given by (3.160), as we saw in section 3.1.

The result (3.163), (3.164) is, of course, what a direct asymptotic expansion gives in a much more parsimonious and general way.

4 General Theory of Effective Conductivity for Random Media

4.1 Introduction and background

In the following sections we will give a more detailed mathematical analysis of homogenization, especially the form it takes for random media. The analysis is independent of dimension so we do not use boldface notation for points x in space. We denote the local conductivity (or diffusivity) by $a(x)$ rather that $D(x)$ because D will denote certain differential operators. We begin with a brief review of the analysis of section 3.1, allowing for greater generality that includes discontinuous coefficients and interfaces.

When $a(x)$ is a given measurable function of $x \in \mathbf{R}^d$ which is periodic of period one in each variable, the solution of the equation

$$-\nabla \cdot \left(a(\frac{x}{\epsilon})\, \nabla u^\epsilon(x) \right) + \alpha\, u^\epsilon(x) = f(x) \;, \qquad x \in \mathbf{R}^d \tag{4.1}$$

converges as $\epsilon \to 0$ to the solution of an equation with constant coefficients, the homogenized problem [3]. Of course equation (4.1) with $\alpha > 0$ and $f(x) \in L^2(\mathbf{R}^d)$ must be interpreted in a suitable weak sense and the convergence of u^ϵ is again in a suitable sense (in $H^1(\mathbf{R}^d)$ weakly and not only in $L^2(\mathbf{R}^d)$ in norm). We are interested in analyzing problems like (4.1) when $a(x)$ is a random function, not necessarily periodic. In the course of analyzing such problems, equation (4.1) will be made precise. In connection with equation (4.1), the general theory of elliptic equations with weakly convergent coefficients, not necessarily periodic or of the form $a(x/\epsilon)$ should be noted [6].

As we noted before, the reason why equations like (4.1) are of interest is clear: one wants to pass from problems with microstructure represented by the rapidly varying coefficients $a(x/\epsilon)$, to asymptotically equivalent problems as $\epsilon \to 0$ which are described by equations with constant or slowly varying coefficients. The analysis is particularly simple for problem (4.1). As in section 3.1 we look for an expansion of the form

$$u^\epsilon(x) = u_0(x, \frac{x}{\epsilon}) + \epsilon u_1(x, \frac{x}{\epsilon}) + \epsilon^2 u_2(x, \frac{x}{\epsilon}) + \cdots \tag{4.2}$$

which is motivated by the form of the coefficients and data in (4.1) as well as experience with multiple scale asymptotics. Inserting (4.2) into (4.1) and noting that the gradient becomes $\nabla_x + \epsilon^{-1}\nabla_y$ when acting on functions of x and $y = x/\epsilon$ we obtain a sequence of problems for $u_0, u_1, u_2, \ldots$ as follows

$$\nabla_y \cdot (a(y)\,\nabla_y u_0) = 0\ , \tag{4.3}$$

$$\nabla_y \cdot (a(y)\nabla_y u_1) + \nabla_y \cdot (a(y)\nabla_x u_0) + \nabla_x \cdot (a(y)\nabla_y u_0) = 0 \tag{4.4}$$

$$\begin{aligned} \nabla_y \cdot (a(y)\nabla_y u_2) \quad &+\nabla_y \cdot (a(y)\nabla_x u_1) + \nabla_x \cdot (a(y)\nabla_y u_1) \\ &+\nabla_x \cdot (a(y)\nabla_x u_0) - \alpha u_0 + f = 0 \end{aligned} \tag{4.5}$$

etc.

From (4.3) we conclude that $u_0 = u_0(x)$ since it is an elliptic equation and dependence of $u_k(x,y)$, $k \geq 0$ on $y = x/\epsilon$ is assumed periodic. Of course, the function $a(y)$ is now assumed smooth, for simplicity, and such that:

$$0 < a_1 \leq a(y) \leq a_2 < \infty \tag{4.6}$$

which is an essential condition.

The next step is to consider (4.4). If we let

$$u_1(x,y) = \sum_{j=1}^{d} \chi^j(y) \frac{\partial u_0(x)}{\partial x_j}\ , \tag{4.7}$$

then $\chi^j(y)$, $j = 1, 2, \ldots, d$ must satisfy

$$\nabla_y \cdot (a(y)) \left(e_j + \nabla_y \chi^j(y) \right) = 0 \ , \qquad j = 1, 2, \ldots, d \ , \tag{4.8}$$

in which e_j is the unit vector in the j^{th} coordinate direction. This of course is nothing but the *cell problem* (3.61) (or (3.49)–(3.52), or (3.37)) with somewhat different notation now. Equation (4.9) has a unique periodic solution $\chi^j(y)$, $j = 1, 2, \ldots, d$, up to an additive constant. If we define

$$q_{ij} = \langle a(e_j + \nabla_y \chi^j) \cdot e_i \rangle \ , \tag{4.9}$$

where $\langle \ \rangle$ denotes cell average, then (q_{ij}) is none other than D^* (cf. (3.62)) in the periodic case of section 3.1.

Consider next (4.5) which is an equation for u_2 as a function of y. The solvability condition for this equation is that the mean value of the inhomogeneous term over a cell vanish. If we use (4.7) in (4.5) and perform the average we obtain the following equation for $u_0(x)$

$$-\sum_{i,j=1}^{d} q_{ij} \frac{\partial^2 u_0(x)}{\delta x_i \delta x_j} + \alpha u_0(x) = f(x) \ , \quad x \in \mathbf{R}^d \ , \quad \alpha > 0 \ . \tag{4.10}$$

This is the effective equation and (q_{ij}) are the effective coefficients.

In section 3 we saw that the calculation of (q_{ij}) is not easy, even in the periodic case. In the random case, only approximate results are known. In this chapter we shall focus attention not on the computation of (q_{ij}) but on the way they arise as coefficients in a limit like the one posed by (4.1). In particular we note that in the periodic case we have obtained an asymptotic expansion

$$u^\epsilon(x) = u_0(x) + \sum_{j=1}^{d} \epsilon \chi^j \left(\frac{x}{\epsilon} \right) \frac{\partial u_0(x)}{\partial x_j} + O(\epsilon^2) \tag{4.11}$$

from which several conclusions can be drawn. First, u^ϵ is close to u_0 in the $L^2(\mathbf{R}^d)$ sense with error of order $\sqrt{\epsilon}$. Second ∇u^ϵ is not close to ∇u_0, which is not surprising if we keep track of the physical meaning of things. What is close to ∇u^ϵ is $\nabla u_0 + \sum_j \nabla \chi^j(x/\epsilon) \dfrac{\partial u_0}{\partial x_j}$ and the error is again of order ϵ is $L^2(\mathbf{R}^d)$. Finally, because of the simplicity of the present problem, higher order terms can be considered to give a full asymptotic expansion, through the Floquet-Bloch expansion (section 3.6) for example.

4.2 Probabilistic formulation

How much of the above goes over to the case of random coefficients? It will be seen that the basic results, the existence of q_{ij} and the convergence of u^ϵ to u_0 in a suitable sense, are preserved provided (4.1) is formulated properly. However, the asymptotic expansion (4.2) cannot be maintained and (4.11) must be modified. In particular the cell problem (4.8), the local microstructure problem, requires careful treatment.

To formulate (4.1) with random coefficients we proceed as follows. Let $(\Omega, \mathcal{F}, P)$ be a probability space. Points $\omega \in \Omega$ will be called realizations or configurations. Let $a(x,\omega)$ be a measurable mapping from $\mathbf{R}^d \times \Omega$ into the real numbers such that

$$0 < a_1 \leq a(x,\omega) \leq a_2 < \infty \quad \text{for all} \quad x \in \mathbf{R}^d \ , \quad \omega \in \Omega \ . \tag{4.12}$$

This function will play the role of coefficients; for each realization ω, the function $a(x,\omega)$, $x \in \mathbf{R}^d$, is given. There are two elements of problem (4.1) with periodic coefficients that must be carried over if a theory that is a suitable generalization is to be found. One is the analog of periodicity which in the random case is statistical homogeneity or stationarity. It means that for any set of points $x_1, x_2, \ldots, x_m$ in $\mathbf{R}^d$ and any vector h, the joint distribution of

$$a(x_1,\omega),\, a(x_2,\omega)\,,\, \ldots,\, a(x_m,\omega)$$

and that of $a(x_1+h,\omega), a(x_2+h,\omega), \ldots, a(x_m+h,\omega)$ is the same. The second is the role of the microstructure parameter ϵ which can enter again in the form $a(x/\epsilon,\omega)$ as in equation (4.1). Both of these can be introduced in more complex forms. But they are necessary in some form.

The equation to be solved is

$$-\nabla \cdot \left(a(\frac{x}{\epsilon},\omega)\, \nabla u^\epsilon(x,\omega) \right) + \alpha\, u^\epsilon(x,\omega) = f(x) \ , \qquad x \in \mathbf{R}^d \ , \ \omega \in \Omega \tag{4.13}$$

that is, for each realization ω, an equation like (4.1) is to be solved. Of course we want only statistical information about u^ϵ in the limit as $\epsilon \to 0$ and that is what we will get. We cannot treat (4.13) realization by realization.

Let $a^\epsilon(x,\omega) = a(x/\epsilon,\omega)$ and let $\langle\ \rangle$ denote average with respect to the measure P over the realizations. Taking averages in (4.13) gives:

$$-\nabla \cdot (\langle a^\epsilon(x)\, \nabla u^\epsilon(x) \rangle) + \alpha \langle u^\epsilon(x) \rangle = f(x) \ , \tag{4.14}$$

from which we see that we need information about $\langle a^\epsilon(x_1)\, u^\epsilon(x_2)\rangle$ since

$$\langle a^\epsilon(x)\,\nabla u^\epsilon(x)\rangle = \lim_{x_2\to x} \nabla_{x_2}\langle a^\epsilon(x)\, u^\epsilon(x_2)\rangle \ .$$

An equation for $\langle a^\epsilon(x_2)\, u^\epsilon(x_2)\rangle$ can be obtained by multiplying (4.13) by $a^\epsilon(x_2)$ and averaging. But this introduces $\langle a^\epsilon(x_2)\, a^\epsilon(x_1)\,\nabla u^\epsilon(x_1)\rangle$ which requires a new equation, etc. It is clear that we have a typical closure problem familiar from nonlinear stochastic problems (nonlinear because u^ϵ is a nonlinear functional of a^ϵ). We will actually show, and this is the main result, that in fact as $\epsilon \to 0$

$$\langle a^\epsilon(x)\,\nabla u^\epsilon(x)\rangle \to q\,\nabla u_0(x)\ ,$$

with $q = (q_{ij})$ suitably computed effective coefficients and $u_0 = \lim\langle u^\epsilon\rangle$. Thus the closure problem posed by (4.13) is solved rigorously in the limit $\epsilon \to 0$.

Let us consider some examples. First, the periodic case is certainly a special case of (4.13) if we take Ω to be the unit torus in $\mathbf{R}^d$, $\mathcal{F}$ the σ-algebra generated by the open sets and P to be Lebesgue measure. Then ω is a point on the unit torus in d-dimensions and we set

$$a(x,\omega) = \tilde{a}(\omega - x)\ ,$$

where $\tilde{a}(\omega)$ is a function on the torus i.e. a periodic function. Problem (4.13) is nothing but (4.1) where the actual location of the origin of coordinates relative to the period cell is chosen randomly within a reference cell. Since the analysis is valid ω by ω, nothing is gained by this randomization.

A more interesting example is the Poisson point process case. Now Ω is the set of infinite sequences of points in $\mathbf{R}^d$, $\omega = (\xi_1, \xi_2, \ldots)$ in which the order is irrelevant, i.e. $\Omega = (\mathbf{R}^d)^\infty$-symmetric. Another convenient way to view Ω is by associating (uniquely) with each ω the point measure $\nu = \sum_j \delta_{\xi_j}(dx)$ where $\delta_y(dx)$ is the Dirac delta measure at y. If A is subset of $\mathbf{R}^d$ then $\nu(A)$ denotes the number of points of ω that fall inside A. For a Poisson process

$$P(\nu(A) = n) = e^{-\lambda|A|}\left(\frac{\lambda|A|}{n!}\right)^n\ , \tag{4.15}$$

where $|A|$ = volume of A and $\lambda > 0$ is a parameter which is called the intensity of the Poisson distribution. It gives the mean number of points per unit volume. Formula (4.15) does not characterize the process completely but its Laplace functional does. If $\phi(x)$ is a positive smooth function of compact support and

$$(\phi, \nu) = \int_{\mathbf{R}^d} \phi(x)\, \nu(dx) = \sum_j \phi(\xi_j) \ ,$$

then

$$E^P \left[e^{-(\phi,\nu)} \right] = \langle e^{-(\phi,\nu)} \rangle = \exp \left[\lambda \int (e^{-\phi(\xi)} - 1)\, d\xi \right] \tag{4.16}$$

is the Laplace functional. Now given this point process, i.e. this probability measures P on the space of point measures on $\mathbf{R}^d$, define

$$a(x,\omega) = \begin{cases} a_2, |x-\xi_j| \le \delta & \text{for some} \quad j \ , \\ a_1, |x-\xi_j| > \delta & \text{for all } j \ . \end{cases} \tag{4.17}$$

We note that the Poisson point process is stationary: $\nu(dx)$ and $\nu(h+dx)$ have the same probability law P. This is easily seen because if $\nu_h(dx) = \nu(h+dx)$ then

$$(\phi, \nu_h) = \int \phi(x)\, \nu(h+dx) = \int \phi(x-h)\, \nu(dx) = (\phi_h, \nu) \ ,$$

where $\phi_h(x) = \phi(x-h)$ and

$$\begin{aligned} \langle e^{-(\phi,\nu_h)} \rangle = \langle e^{-(\phi_h,\nu)} \rangle \quad &= \exp \left[\lambda \textstyle\int (e^{-\phi(\xi-h)} - 1)\, d\xi \right] \\ &= \exp \left[\lambda \textstyle\int (e^{-\phi(\xi)} - 1)\, d\xi \right] \\ &= \langle e^{-(\phi,\nu)} \rangle \ , \end{aligned}$$

and so the Laplace functional, hence the measure P, does not depend on h. Since $a(x,\omega)$ is a random function which is a functional of the Poisson process, it is itself stationary.

The random function (4.17) gives for example the conductivity of a medium with spherical inclusions placed randomly according to a Poisson process (with $d=3$). Notice that the spheres are allowed to overlap, so the Poisson process is not a particularly useful process for modeling a random conducting medium. Overlap will occur even if $4/3\,\pi\delta^3\lambda$, which measures the volume fraction occupied by the spheres, is small. Nevertheless the example (4.17) is instructive and we will use it. In particular we note that the scaling

$$a(x,\omega) = a(\frac{x}{\epsilon}, \omega)$$

can be achieved in another equivalent way that is perhaps better motivated. Suppose that we set

$$\lambda = \epsilon^{-d} \tilde{\lambda} \ , \qquad \delta = \epsilon \tilde{\delta} \ ,$$

and denote the resulting random function a by $a^\epsilon(x,\omega)$. Suppose we replace ω by $\epsilon\omega$ or ν by $\nu(\epsilon\, dx) = \nu^\epsilon(dx)$. Then

$$\begin{aligned}\langle e^{-(\phi,\nu^\epsilon)}\rangle &= \exp\left[\epsilon^{-d}\tilde{\lambda}\int \left(e^{-\phi(\xi/\epsilon)}-1\right)\, d\xi\right]\\ &= \exp\left[-\tilde{\lambda}\int\left(e^{-\phi(\xi)}-1\right)\, d\xi\right] \ .\end{aligned}$$

Hence ν^ϵ with law P which is Poisson with parameter $\epsilon^{-d}\tilde{\lambda}$ is statistically equivalent to the Poisson point process with parameter $\tilde{\lambda}$. But then

$$\begin{aligned}\hat{a}^\epsilon(x,\omega) &= \begin{cases} a_2 \ , \ |x-\epsilon\xi_j| \le \epsilon\tilde{\delta} & \text{for some } j \ , \\ a_1 \ , \ |x-\epsilon\xi_j| > \epsilon\delta & \text{for some } j \ , \end{cases}\\ &= \begin{cases} a_2 \ , \ |\frac{x}{\epsilon}-\xi_j| \le \tilde{\delta} & \text{for some } j \ , \\ a_1 \ , \ |\frac{x}{\epsilon}-\xi_j| > \tilde{\delta} & \text{for all } j \ , \end{cases}\\ &= a\left(\tfrac{x}{\epsilon},\omega\right) \ ,\end{aligned}$$

where the last equality is in the sense of statistical equivalence (i.e. in distribution) and $a(x,\omega)$ is as in (4.17) with $\delta = \tilde{\delta}$ and $\lambda = \tilde{\lambda}$ in the Poisson law.

We impose a convenient structure on the probability space $(\Omega, \mathcal{F}, P)$ in order to carry out the asymptotic analysis of (4.13). We shall assume that there is a group of transformations

$$\tau_x \colon \Omega \to \Omega \ , \quad x \in \mathbf{R}^d \tag{4.18}$$

which is one-to-one and preserves P. This means that if G is any set in $\mathcal{F}$ then

$$P(\tau_x^{-1}G) = P(G) \ ,$$

where

$$\tau_x^{-1}G = \{\omega \in \Omega \mid \tau_x\omega \in G\} \ .$$

The group property is: $\tau_x\tau_y = \tau_{x+y}$, $x,y \in \mathbf{R}^d$. Now we assume that the coefficient function $a(x,\omega)$ defined on $\mathbf{R}^d \times \Omega$ has the form

$$a(x,\omega) = \tilde{a}(\tau_{-x}\,\omega) \ , \tag{4.19}$$

where $\tilde{a}(\omega)$ is a given function on Ω satisfying (4.12). Notice that by putting this structure on $(\Omega, \mathcal{F}, P)$ and defining $a(x,\omega)$ as in (4.19), we are assured that it is stationary.

In the periodic case ω is a point in the period cell, obviously $\tau_x\omega = \omega + x$ with addition being modulo one. This is one to one and preserves Lebesgue measure. Moreover the coefficient function $a(x,\omega) = \tilde{a}(\tau_{-x}\omega)$ does have the correct form.

In the Poisson case $\omega = (\xi_1, \xi_2, \ldots)$ and we put

$$\tau_x\omega = (\xi_1 + x,\, \xi_2 + x,\, \ldots) \tag{4.20}$$

which again leaves the Poisson measure invariant as we verified already. Obviously $a(x,\omega)$ of (4.17) has the form

$$a(x,\omega) = \tilde{a}(\tau_{-x}\omega)\ , \tag{4.21}$$

where

$$\tilde{a}(\omega) = \begin{cases} a_2\ , & |\xi_j| \le \delta \quad \text{for some } j\ , \\ a_1\ , & |\xi_j| > \delta \quad \text{for some } j\ . \end{cases} \tag{4.22}$$

Returning to the general setup, it will be convenient to introduce some notation. Let

$$\mathcal{H} = L^2(\Omega, \mathcal{F}, P) \tag{4.23}$$

be the Hilbert space of real functions on Ω with inner produced denote by

$$(\tilde{f}, \tilde{g}) = E^P\{\tilde{f}\,\tilde{g}\} = \int_\Omega \tilde{f}(\omega)\,\tilde{g}(\omega)\,P(d\omega) = \langle \tilde{f}\,\tilde{g}\rangle\ . \tag{4.24}$$

On this Hilbert space we define a unitary group of operators T_x: $\mathcal{H} \to \mathcal{H}$ by

$$(T_x\tilde{f})(\omega) = \tilde{f}(\tau_{-x}\omega)\ , \qquad x \in \mathbf{R}^d\ . \tag{4.25}$$

The unitarity follows from the translation invariance of P and the one-one nature of τ_x. Since the operators T_x form a group we can define their infinitesimal generator by

$$\left.\frac{\partial}{\partial x_i} T_x\tilde{f}\right|_{x=0} = D_i\tilde{f}\ , \qquad i = 1, 2, \ldots, d\ , \tag{4.26}$$

where the derivative is in the sense of the norm in $\mathcal{H}$ and (4.26) is defined for $\tilde{f} \in \mathcal{D}_i$, the domains of the generators. These sets $\mathcal{D}_i \subset \mathcal{H}$ are densely defined and the set

$$\mathcal{H}_i = \bigcap_{i=1}^d \mathcal{D}_i\ , \tag{4.27}$$

equipped with the inner product

$$((\tilde{f}, \tilde{g})) = (\tilde{f}, \tilde{g}) + \sum_{i=1}^d (D_i\tilde{f}, D_i\tilde{g})\ , \tag{4.28}$$

is a Hilbert subspace of $\mathcal{H}$. We shall call it the Sobolev space $\mathcal{H}_1$ by analogy with the usual case of functions and derivatives in $\mathbf{R}^d$.

Let us look at what the above definitions mean in the examples. In the periodic case $L^2(\Omega, \mathcal{F}, P)$ is simply the Hilbert space of square integrable periodic functions. The operators T_x are the usual translation operators and the generators D_i are the partial derivatives $\partial/\partial\omega_i$. Hence $\mathcal{H}_1$ is the usual Sobolev space of functions on the torus with square integrable derivatives.

In the Poisson case, $\mathcal{H}$ is the Hilbert space of functions on Ω with inner product as in (4.24). A dense set of functions in $\mathcal{H}$ can be obtained as follows. Let $\phi_1, \phi_2, \ldots$ be a countable dense set of functions on $\mathbf{R}^d$ (such as the Hermite functions). Let F be a smooth function from $\mathbf{R}^m \to \mathbf{R}$. Put

$$\tilde{f}(\omega) = F(\,(\phi_{j_1}, \nu), (\phi_{j_2}, \nu), \ldots, (\phi_{j_m}, \nu)\,)\ . \tag{4.29}$$

As we vary the index set $j_1, j_2, \ldots, j_m$ and the function F, we obtain a class of functions $\tilde{f}$ that are dense in the space of continuous functions on Ω and hence in $\mathcal{H}$. The translation operators T_x are well defined on functions of the form (4.29) and so are the D_i. In fact

$$(D_i\tilde{f})(\omega) = \sum_{k=1}^{m} \frac{\partial F}{\partial z_k}\left((\phi_{j_1}, \nu), \ldots, (\phi_{j_m}, \nu)\right)\left(\frac{\partial}{\partial x_i}\phi_{j_k}, \nu\right)\ , \tag{4.30}$$

and the functions (4.29) are dense in $\mathcal{H}_1$ as well provided F and the $\{\phi_j\}$ are smooth.

Before going to the analysis of (4.13) as $\epsilon \to 0$, we need one more hypothesis which is as follows:

$$\text{The action of } \tau_x \text{ on } \Omega \text{ is ergodic with respect to } P\ . \tag{4.31}$$

This means that if G is any set in $\mathcal{F}$ that invariant under τ_x, i.e. $\tau_x^{-1}G \supset G$ then G has probability zero or one.

4.3 The effective conductivity

Let us look at the periodic problem (4.1). Let

$$z^\epsilon(x) = u^\epsilon(x) - u_0(x) - \sum_{j=1}^{d} \epsilon\chi^j\left(\frac{x}{\epsilon}\right)\frac{\partial u_0(x)}{\partial x_j}\ , \tag{4.32}$$

where $\chi^j(y)$ are solutions of the cell problem (4.8). We have

$$
\begin{aligned}
-\nabla\cdot\left(a(\frac{x}{\epsilon})\nabla z^\epsilon\right)+\alpha z^\epsilon &= \nabla\cdot\left[a(\frac{x}{\epsilon})\nabla(u_0-\sum_{j=1}^{d}\frac{\epsilon\chi^j\partial u_0}{\partial x_j})\right]\\
&\quad -\alpha(u_0+\sum_{j=1}^{d}\epsilon\chi^j\frac{\partial u_0}{\partial x_j})+f\\
&= \frac{1}{\epsilon}\sum_j\nabla_y\cdot\left[a(y)\,(e_j+\nabla_y\chi^j)\right]\frac{\partial u_0}{\partial x_j}\Big|_{y=x/\epsilon} \qquad (4.33)\\
&\quad +\sum_j\nabla_x\cdot\left[a(y)\,(e_j+\nabla_y\chi^j)\frac{\partial u_0}{\partial x_j}\right]\Big|_{y=x/\epsilon}\\
&\quad +\epsilon\sum_j\nabla_x\cdot\left[a(y)\,\chi^j(y)\frac{\partial u_0}{\partial x_j}\right]\Big|_{y=x/\epsilon}\\
&\quad -\alpha u_0-\alpha\sum_j\epsilon\chi^j\frac{\partial u_0}{\partial x_j}+f\ .
\end{aligned}
$$

The first term on the right side vanishes because the χ^j satisfy the cell problem (4.33). The order one in ϵ terms combine via (4.10) to give

$$
\sum_{i,j=1}^{d}\left[a(y)\left(\delta_{ij}+\frac{\partial y^j(y)}{\partial y_i}\right)-q_{ij}\right]\frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j}\ . \qquad (4.34)
$$

Note that the term in brackets in (4.34) has mean zero. Denote it by $\hat{q}_{ij}(y)$. Then we rewrite (4.33) in the form

$$
\begin{aligned}
-\nabla\cdot\left(a(\frac{x}{\epsilon})\nabla z^\epsilon\right)+\alpha z^\epsilon &= \sum_{i,j=1}^{d}\hat{q}_{ij}(\frac{x}{\epsilon})\frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j}\\
&\quad +\epsilon\sum_{ij}a(\frac{x}{\epsilon})\,\chi^j(\frac{x}{\epsilon})\frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j} \qquad (4.35)\\
&\quad -\epsilon\sum_j\alpha^j(\frac{x}{\epsilon})\frac{\partial u_0(x)}{\partial x_j}\ .
\end{aligned}
$$

From (4.35) we deduce easily that

$$
\int_{\mathbf{R}^d}\left[(\nabla z^\epsilon)^2+(z^\epsilon)^2\right]\,dx\to 0\quad \epsilon\quad \text{as}\quad e\downarrow 0 \qquad (4.36)
$$

which gives us the convergence theorem for (4.1) in the periodic case. The only point that must be clarified in passing from (4.35) to (4.36) is why the first term on the right of (4.35) which appears to be of order one in ϵ, is small. This is seen by noting that since

$\hat{q}_{ij}(y)$ are periodic and have mean zero we can always find functions $Q_{ij}^k(y)$ also periodic such that

$$\frac{\partial}{\partial y_k}(Q_{ij}^k(y)) = q_{ij}(y) \quad \text{(summation on } k) \ . \tag{4.37}$$

Substituting this into the right side of (4.35), integrating by parts and using (4.6) gives the convergence result (4.36) which is in fact of order ϵ.

How should this be modified in order that the random case be accommodated? Obviously we should first try to write $u^\epsilon(x,\omega)$, the solution of (4.13), in the form

$$u^\epsilon(x,\omega) = u_0(x) + \epsilon \sum_{j=1}^{d} \chi^j(\frac{x}{\epsilon},\omega)\frac{\partial u_0(x)}{\partial x_j} + z^\epsilon(x,\omega) \ . \tag{4.38}$$

The analysis of the periodic case tells us that $\chi^j(y,\omega)$ should satisfy the cell problem

$$\nabla_y \cdot [a(y,\omega)(e_j + \nabla_y \chi^j(y,\omega))] = 0 \ , \quad y \in \mathbf{R}^d \ , \quad \omega \in \Omega \ , \quad j - 1, 2, \ldots, d \ . \tag{4.39}$$

Does this problem have a solution $\chi^j(y,\omega)$ which is a stationary random function? This is not at all obvious and it is in fact false in general.

4.4 The abstract cell problem

To begin the analysis of (4.39) we note that if $\chi^j(y,\omega)$ is to be a stationary solution it should have the form

$$\chi^j(y,\omega) = \tilde{\chi}^j(\tau_{-y}\omega) \ . \tag{4.40}$$

Now for any function of the form

$$f(y,\omega) = \tilde{f}(\tau_{-y}\omega) \ ,$$

we note that the definition (4.26) gives

$$\frac{\partial f(y,\omega)}{\partial y_j} = (D_j\tilde{f})(\tau_{-y}\omega) \ . \tag{4.41}$$

The equality being valid in $\mathcal{H}$ for functions $\tilde{f}$ that belong to $\mathcal{H}_1$. With this observation (4.39) can be transformed into a problem for $\tilde{\chi}^i(\omega)$ which has the form

$$\sum_i D_i \left[\tilde{a}(\omega)(\delta_{ij} + D_i\tilde{\chi}^j(\omega))\right] = 0 \ , \qquad j = 1, 2, \ldots, d \ . \tag{4.42}$$

This is the *abstract* cell problem in which x dependence has been removed.

Clearly the problem (4.42) should be interpreted as a variational problem in the abstract Sobolev space $\mathcal{H}_1$. The variational form is this. Find $\tilde{\chi}^j(\omega)$ in $\mathcal{H}_1$ such that:

$$\sum_i \int_\Omega \tilde{a}(\omega)\,(\delta_{ij} + D_i\tilde{\chi}^j(\omega)\,)\,D_i\tilde{\phi}(\omega)\,P(d\omega) = 0\ , \quad j = 1, 2, \ldots, d\ ,$$

for all $\tilde{\phi} \in \mathcal{H}_1$. This can be rewritten as

$$\int_\Omega \tilde{a}(\omega) \sum_i D_i\tilde{\chi}^j(\omega)\,D_i\tilde{\phi}(\omega)\,P(d\omega) = -\int_\Omega \tilde{a}(\omega)\,D_j\,\tilde{\phi}(\omega)\,P(d\omega)\ . \tag{4.43}$$

Unfortunately the abstract cell problem (4.43) does not have a solution because the bilinear form on the left is not coercive in $\mathcal{H}_1$ which has inner product (4.23). Recall that in the periodic case where Ω is the unit torus, the coercivity of the bilinear form is obtained via the Poincaré inequality which does not hold, of course, in the general abstract Sobolev space $\mathcal{H}_1$.

There are a couple of ways available for getting out of this difficulty, both of which are interesting. One is to realize that (4.43) does indeed have a solution but not in the form $\tilde{\chi}^j$. Rather in the form $\tilde{\psi}_i^j(\omega)$ which formally replaces $D_i\tilde{\chi}^j(\omega)$. The abstract gradient of $\tilde{\chi}^j(\omega)$ is a configuration function but $\tilde{\chi}^j$ itself is not. Said another way: a stationary solution $\chi^j(y,\omega)$ of (4.39) cannot be found but we can find stationary random functions $\psi_i^j(y,\omega)$ such that $\frac{\partial}{\partial y_i}\chi^j(y,\omega) = \psi_i^j(y,\omega)$. Of course $\chi^j(y,\omega)$ will not be stationary. In fact the problem for $\psi_i^j(y,\omega)$ is nothing other than (3.48)–(3.51) with $e = e_j$ where $G_i(y,\omega) = \psi_i^j(y,\omega)$. This is the reason problem (3.49)–(3.52) was written for the fields F, G directly rather than the gradient.

The second way is as follows. We can always regularize (4.43) by defining $\chi_\beta^j(y,\omega) = \tilde{\chi}_\beta^j(\tau_{-y}\omega)$ to be the solution of

$$\begin{aligned} \textstyle\int_\Omega \tilde{a}(\omega) \sum_i D_i\tilde{\chi}_\beta^j(\omega)\,D_i\tilde{\phi}(\omega)\,P(d\omega) + \beta \int_\Omega \tilde{\chi}_\beta^j(\omega)\,\tilde{\phi}(\omega)\,P(d\omega) \\ = -\textstyle\int_\Omega \tilde{a}(\omega)\,D_j\tilde{\phi}(\omega)\,P(d\omega)\ , \end{aligned} \tag{4.44}$$

$\forall\,\tilde{\phi} \in \mathcal{H}_1$, $j = 1, 2, \ldots, d$, $\beta > 0$. This problem has a unique solution in $\mathcal{H}_1$ by the Lax-Milgram lemma [27]. Before analyzing (4.44) further, especially the behavior of $\tilde{\chi}_\beta^j$ as $\beta \to 0$, let us look at the expansion (4.38) with $\chi^j(y,\omega)$ replaced by $\chi_\beta^j(y,\omega)$.

We write (4.38) in the form

$$u^\epsilon(x,\omega) = u_0(x) + \epsilon \sum_{j=1}^{d} \chi_\beta^j(\frac{x}{\epsilon},\omega)\frac{\partial u_0(x)}{\partial x_j} + z^\epsilon(x,\omega)\ , \tag{4.45}$$

and attempt to choose $\beta = \beta(\epsilon)$ so that the error z^ϵ can be still estimated. Obviously we must have

$$\langle (u^\epsilon - u_0)^2 \rangle \to 0 \quad \text{as} \quad \epsilon \to 0 \ . \tag{4.46}$$

From (4.45) this means that we must have

$$\epsilon^2 \langle (\chi_\beta^j)^2 \rangle \to 0 \quad \text{as} \quad \epsilon \to 0 \ , \ \ j = 1, 2, \ldots, d \ , \tag{4.47}$$

for a suitable $\beta = \beta(\epsilon)$. On the other hand, if u^ϵ has the form (4.45) then the $O(1/\epsilon)$ term on the right side of (4.33) does not vanish but, by (4.44) is equal to

$$\frac{\beta}{\epsilon} \sum_{j=1}^{d} \chi_\beta^j \left(\frac{x}{\epsilon}, \omega \right) \frac{\partial u_0(x)}{\partial x_j} \ .$$

This means that we must require that

$$(\frac{\beta}{\epsilon})^2 \langle (\chi_\beta^j)^2 \rangle \to 0 \quad \text{as} \quad \epsilon \to 0 \ , \ \ j = 1, 2, \ldots, d \ , \tag{4.48}$$

for a suitable $\beta = \beta(\epsilon)$. Both (4.47) and (4.48) hold provided we choose $\beta = \beta(\epsilon)$ so that

$$\frac{\beta^2}{\epsilon^2} = \epsilon^2 \quad \text{or} \quad \beta = \epsilon^2 \ , \tag{4.49}$$

and then we have to show that

$$\lim_{\beta \to 0} \beta \langle (\chi_\beta^j)^2 \to 0 \quad \text{as} \quad \beta \downarrow 0 \ , \ \ j = 1, 2, \ldots, d \ . \tag{4.50}$$

Let us show that the solution $\tilde{\chi}_\beta^j$ of (4.44) satisfies (4.50) since by stationarity we can replace χ_β^j by $\tilde{\chi}_\beta^j$ in (4.50). If we let $\tilde{\phi} = \tilde{\chi}_\beta^j$ in (4.44) we get

$$\sum_i \langle \tilde{a} D_i \tilde{\chi}_\beta^j D_i \tilde{\chi}_\beta^j \rangle + \beta \langle (\tilde{\chi}_\beta^j)^2 \rangle = - \langle \tilde{a} D_j \tilde{\chi}_\beta^j \rangle \ .$$

From the uniform bounds (4.6) on a or $\tilde{a}$ we get the estimates

$$\sum_i \langle (D_i \tilde{\chi}_\beta^j)^2 \rangle \leq C \ , \tag{4.51}$$

$$\beta \langle (\tilde{\chi}_\beta^j)^2 \rangle \leq C \ , \tag{4.52}$$

where C denotes a constant independent of β. From (4.51) we deduce that as $\beta \to 0$, along a subsequence possibly,

$$D_i \tilde{\chi}_\beta^j \to \psi_i^j \text{ weakly in } \mathcal{H} \ . \tag{4.53}$$

Passing to the limit in (4.44) we get then

$$\langle \tilde a \sum_i \tilde\psi_i^j D_i \tilde\phi\rangle = -\langle \tilde a\, D_j\, \tilde\phi\rangle\ , \qquad \forall\, \tilde\phi \in \mathcal{H}_1\ . \tag{4.54}$$

Letting $\tilde\phi = \tilde\chi_\beta^j$ in (4.54) and letting β tend to zero again we get also

$$\langle \tilde a \sum_i \tilde\psi_i^j \tilde\psi_i^j\rangle = -\langle \tilde a\, \tilde\psi_j^j\rangle\ . \tag{4.55}$$

We want to prove (4.50). Putting $\tilde\phi = \tilde\chi_\beta^j$ in (4.44) and taking upper limit as $\beta \to 0$ gives

$$\overline{\lim_{\beta\downarrow 0}}\langle \tilde a \sum_i (D_i \tilde\chi_\beta^j)^2\rangle + \overline{\lim_{\beta\downarrow 0}}\beta\langle(\tilde\chi_\beta^j)^2\rangle = -\langle \tilde a\, \tilde\psi_j^j\rangle\ . \tag{4.56}$$

From the weak convergence in (4.53) we deduce that

$$\underline{\lim_{\beta\downarrow 0}}\langle \tilde a \sum_i (D_i\, \tilde\chi_\beta^j)^2\rangle \ge \langle \tilde a \sum_i (\tilde\psi_i^j)^2\rangle\ . \tag{4.57}$$

This is seen from the fact that

$$\langle \tilde a \sum_i (D_i \tilde\chi_\beta^j)^2\rangle \ge \frac{\langle \tilde a \sum_i D_i \tilde\chi_\beta^j D_i \tilde\phi\rangle^2}{\langle \tilde a \sum_i D_i \tilde\phi D_i \tilde\phi\rangle}\ ,$$

for all $\tilde\phi \in \mathcal{H}_1$. Taking the *liminf* and then the supremum over $\tilde\phi \in \mathcal{H}_1$ gives (4.57). Using now (4.57) in (4.56) we get

$$\overline{\lim}\, \beta\langle(\tilde\chi_\beta^j)^2\rangle \le -\langle \tilde a\, \tilde\psi_j^j\rangle - \langle \tilde a \sum_i (\tilde\psi_i^j)^2\rangle = 0$$

by (4.55) and so (4.50) has been proven.

4.5 Convergence of random homogenization

Let us return to the error equation (4.33), rewritten with $z^\epsilon = z^\epsilon(x,\omega)$ and χ^j replaced by $\chi_\beta^j(x/\epsilon,\omega)$ with $\beta = \epsilon^2$. We have:

$$\begin{aligned}
&-\nabla\cdot[a(\frac{x}{\epsilon},\omega)\,\nabla z^\epsilon(x,\omega)] + \alpha\, z^\epsilon(x,\omega) \\
&\quad = \frac{\beta}{\epsilon}\sum_j \chi_\beta^j(\frac{x}{\epsilon},\omega)\frac{\partial u_0(x)}{\partial x_j} + \sum_{i,j}\hat q_{ij}^\beta(\frac{x}{\epsilon},\omega)\frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j} \\
&\quad\quad + \epsilon\sum_{i,j} a(\frac{x}{\epsilon},\omega)\,\chi_\beta^j(\frac{x}{\epsilon},\omega)\frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j} - \epsilon\sum_j \alpha\,\chi_\beta^j(\frac{x}{\epsilon},\omega)\frac{\partial u_0(x)}{\partial x_j}\ .
\end{aligned} \tag{4.58}$$

Multiplying (4.58) by z^ϵ and integrating over x and ω gives ($a^\epsilon = a(x/\epsilon, \omega)$):

$$\begin{aligned}
&\textstyle\int dx \langle a^\epsilon (\nabla z^\epsilon)^2\rangle + \alpha \int dx \langle (z^\epsilon)^2 \rangle \\
&\quad = \tfrac{\beta}{\epsilon} \textstyle\int \langle \sum_j \chi_\beta^j(\frac{x}{\epsilon}, \omega) \frac{\partial u_0(x)}{\partial x_j}\, z^\epsilon(x,\omega)\rangle\, dx \\
&\qquad + \textstyle\int \displaystyle\sum_{i,j} \langle \hat{q}_{ij}^\beta(\frac{x}{\epsilon}, \omega) \frac{\partial^2 u_0(x)}{\partial x_i\, \partial x_j}\, z^\epsilon(x,\omega)\rangle\, dx \\
&\qquad + \epsilon \int \sum_{i,j} \langle a(\frac{x}{\epsilon}, \omega)\, \chi_\beta^j(\frac{x}{\epsilon}, \omega) \frac{\partial^2 u_0(x)}{\partial x_i\, \partial x_j}\, z^\epsilon(x,\omega)\rangle\, dx \\
&\qquad - \epsilon \int \sum_i \alpha \langle \chi_\beta^j(\frac{x}{\epsilon}, \omega)\, \frac{\partial u_0(x)}{\partial x_j}\, z^\epsilon(x,\omega)\rangle\, dx \ ,
\end{aligned} \tag{4.59}$$

where, as in (4.34)

$$\hat{q}_{ij}^\beta(y,\omega) = a(y,\omega)\,(\delta_{ij} + \frac{\partial \chi_\beta^j(y,\omega)}{\partial y_i}) - q_{ij} \tag{4.60}$$

and

$$q_{ij} = \langle a(y,\omega)\,(\delta_{ij} + \psi_i^j(y,\omega)\rangle \ . \tag{4.61}$$

Clearly $\psi_i^j(y,\omega) = \tilde{\psi}_i^j(\tau_{-y}\omega)$ with $\tilde{\psi}_i^j$ the unique solution of (4.54). The uniqueness follows easily from (4.54) by contradiction and the use of the ellipticity hypothesis (4.6). Namely, the difference of any two solutions of (4.54) must satisfy

$$\langle \sum_i \tilde{\psi}_i^j\, D_i\, \tilde{\phi}\rangle = 0 \ , \qquad \forall\, \tilde{\phi} \in \mathcal{H}_1 \ .$$

Choosing $\tilde{\phi} = \tilde{\chi}_\beta^j$ and passing to the limit gives the uniqueness.

From (4.38) and the usual uniform bounds on the norms of u^ϵ and ∇u^ϵ we know that

$$\int \left[\langle (\nabla z^\epsilon)^2\rangle + \langle (z^\epsilon)^2\rangle \right] dx \le C \ , \tag{4.62}$$

where C is a constant independent of ϵ. We can also take the limit $\epsilon \to 0$ in (4.59). Because of (4.50) and (4.62) we see that

$$\begin{aligned}
&\overline{\lim_{\epsilon \downarrow 0}} \int \left[\langle (\nabla z^\epsilon)^2\rangle + \langle (z^\epsilon)^2\rangle \right] \\
&\le \overline{\lim_{\epsilon \downarrow 0}} \int \sum_{i,j} \langle \hat{q}_{ij}(\frac{x}{\epsilon}, \omega)\, z^\epsilon(x,\omega)\rangle \frac{\partial^2 u_0(x)}{\partial x_i\, \partial x_j}\, dx \ ,
\end{aligned} \tag{4.63}$$

with $\hat{q}_{ij}$ given by

$$\hat{q}_{ij}(y,\omega) = a(y,\omega)\,(\delta_{ij} + \psi_i^j(y,\omega)\,) - q_{ij} \ , \tag{4.64}$$

so that $\hat{q}_{ij}$ are stationary and

$$\langle \hat{q}_{ij} \rangle = 0 \ . \tag{4.65}$$

It remains therefore to show that the right side of (4.63) is zero.

The ergodicity hypothesis (4.31) has not been used yet. It will be used now in the following way. First we note that the ergodicity hypothesis (4.31) is equivalent to the statement that if $\tilde{f}(\omega)$ is a function in $\mathcal{H}$ such that

$$(T_x\tilde{f})(\omega) = \tilde{f}(\omega)\ , \qquad x \in \mathbf{R}^d\ ,\ P \text{ a.e.}$$

that is, if $\tilde{f}(\omega)$ is an invariant function, then $\tilde{f}$ = constant P a.e. For the unitary group of operation T_x on $\mathcal{H}$ we also have the spectral representation

$$T_x = \int_{\mathbf{R}^d} e^{ik\cdot x}\, U(dk)\ , \tag{4.66}$$

where $U(dk)$ are projection valued measures on $\mathcal{H}$. Another equivalent form of ergodicity is that the projection operator $U(\{0\})$ to zero frequency is one dimensional and contains the constants only.

We proceed as follows. Let

$$\tilde{q}_{ij}(\tau_{-y}\omega) = \hat{q}_{ij}(y,\omega)\ , \tag{4.67}$$

so that $\tilde{q}_{ij}(\omega)$ are functions on Ω with zero mean. Define

$$h^\ell_{ij}(y,\omega) = \int_{\mathbf{R}^d} (e^{ik\cdot x} - 1)\frac{-ik_\ell}{|k|^2} U(dk)\, \tilde{q}_{ij}(\omega)\ . \tag{4.68}$$

Now

$$\sum_{\ell=1}^d \frac{\partial}{\partial y_\ell}\, h^\ell_{ij}(y,\omega) = \int e^{ik\cdot x}\, U(dk)\, \tilde{q}_{ij}(\omega) = \hat{q}_{ij}(y,\omega)\ . \tag{4.69}$$

Moreover we have that

$$\lim_{\epsilon\downarrow 0}\langle(\epsilon h^\ell_{ij}(\frac{x}{\epsilon},\omega))^2\rangle = 0\ . \tag{4.70}$$

To see why (4.70) holds, note that

$$\langle(\epsilon h^\ell_{ij}(\frac{x}{\epsilon},\omega)\,)^2\rangle = \int_{\mathbf{R}^d} \frac{|e^{ix\cdot(k/\epsilon)} - 1|^2}{|k/\epsilon|^2}\, \frac{k_\ell k_\ell}{|k|^2}\, \widehat{R}_{ij}(dk)\ , \tag{4.71}$$

where

$$\widehat{R}_{ij}(dk) = \langle U(dk)\tilde{q}_{ij}, \tilde{q}_{ij}\rangle. \tag{4.72}$$

By the hypothesis of ergodicity we know that $\widehat{R}_{ij}(\{0\}) = 0$ since $\tilde{q}_{ij}$ has mean zero and the only invariant functions are constants. The Lebesgue dominated convergence theorem can now be applied to (4.71) and it gives (4.70).

To complete the proof that the right side of (4.63) is zero we replace $\hat{q}_{ij}$ by (4.69) and integrate by parts. Thus:

$$
\begin{aligned}
&\int \sum_{ij} \langle \hat{q}_{ij}(\frac{x}{\epsilon},\omega)\, z^\epsilon(x,\omega)\rangle \frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j}\,dx \\
&= \int \sum_{ij} \langle \sum_\ell \epsilon \frac{\partial}{\partial x_i}\, h^\ell_{ij}(\frac{x}{\epsilon},\omega)\, z^\epsilon(x,\omega)\rangle \frac{\partial^2 u_0(x)}{\partial x_i \partial x_j}\,dx \\
&\quad + \int \sum_{i,j,\ell} \langle \epsilon\, h^\ell_{ij}(\frac{x}{\epsilon},\omega) \frac{\partial x^\epsilon}{\partial x_\ell}(x,\omega)\rangle \frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j}\,dx \\
&\quad - \int \sum_{i,j\ell} \langle \epsilon h^\ell_{ij}(\frac{x}{\epsilon},\omega)\, z^\epsilon(x,\omega)\rangle \frac{\partial^3 u_0(x)}{\partial x_i\,\partial x_j\,\partial x_\ell}\,dx\ .
\end{aligned}
$$

The estimate (4.62) that holds uniformly in ϵ and (4.70) show that the right side of (4.63) is zero.

We can summarize the above by saying that the solution of

$$
\begin{gathered}
-\nabla\cdot\big(a(\tfrac{x}{\epsilon},\omega)\,\nabla u^\epsilon(x,\omega)\big) + \alpha u^\epsilon(x,\omega) = f(x)\ , \quad \alpha > 0\ , \quad x\in \mathbf{R}^d\ , \\
\omega\in\Omega\ , \quad f\in C_0^\infty(\mathbf{R}^d)\ ,
\end{gathered}
\tag{4.73}
$$

interpreted in weak or variational form, converges to the solution $u_0(x)$ of

$$
-\sum_{i,j} q_{ij} \frac{\partial^2 u_0(x)}{\partial x_i\,\partial x_j} + \alpha u_0(x) = f(x)\ , \tag{4.74}
$$

where q_{ij} is defined by (4.61). The sense of the convergence is mean square:

$$
\int_{\mathbf{R}^d} dx \langle (u^\epsilon(x,\omega) - u_0(x)\,)^2\rangle \to 0\ . \tag{4.75}
$$

We also have the stronger result that if

$$
z^\epsilon(x,\omega) = u^\epsilon(x,\omega) - u_0(x) - \epsilon \sum_{j=1}^d \chi^j_{\epsilon^2}\left(\frac{x}{\epsilon},\omega\right) \frac{\partial u_0(x)}{\partial x_j}\ , \tag{4.76}
$$

then

$$
\int_{\mathbf{R}^d} \langle (\nabla z^\epsilon)^2 + (z^\epsilon)^2\rangle \to 0 \quad \text{as} \quad \epsilon\to 0\ . \tag{4.77}
$$

4.6 Computational issues

The main point about homogenization in random media is that the simple multiple scale expansion (sections 3.1 and 4.3) is not in fact an expansion and the error term z^ϵ just barely makes it to zero as ϵ tends to zero. The corrector term $\sum_{j=1}^d \epsilon\chi^j\left(\frac{x}{\epsilon}\right)\frac{\partial u_0(x)}{\partial x_j}$ in (4.32) is an essential part of the solution, especially in the form it takes in section 4.4 where χ^j is replaced by χ^j_β. The cell problem, which is the central part of any kind of analysis, is best written in the form (2.3-2.6) with the effective coefficient given by (2.7) or (2.8). Best means mathematically best (as we saw in section 4.4) and physically best because in this form the cell problem is the obvious thing to consider in an effective medium theory. What about numerical computations? This is an important issue that requires special consideration.

For a periodic structure the cell problem, in the form of section 3.1.1 or 3.1.4 for example, is a standard elliptic boundary value problem that can be solved routinely by finite element methods. If the microscopic diffusivity $D(\mathbf{y})$ (denoted by a in section 4) is a complicated function that takes very large and very small values, corresponding to a high-contrast medium, the finite element method will require a lot of resolution and will be expensive. There are special approximation techniques available for high contrast materials [32, 31] but it is not clear how to use them systematically to improve computational methods.

For random structures the obvious and frequently used idea is to approximate the infinite cell problem (2.3-2.6) by a periodic one with large period so that a 'typical' random part is included. We know theoretically that the stationary and ergodic structure of the coefficients suffices for the solution of the periodized cell problem to converge to the random one, in the sense that the effective coefficients will converge. But we have no idea how fast the coefficients will converge and what controls the rate of convergence. To see why this is a very difficult problem consider the example of spherical inclusions discussed in detail in sections 3.2, 3.3 and 3.4. Given a small volume fraction β, say less than 1%, and independent sphere placements, how big a period cell should we have to use to recover accurately by numerical computations the approximate formula (3.59)

$$\frac{D^* - D_1}{D^* + 2D_1} = \beta \frac{D_2 - D_1}{D_2 + 2D_1} \ . \tag{4.78}$$

for the effective diffusivity D^*? How does the size of the periodized problem depend on the volume fraction if the spherical inclusions are not allowed to overlap? It is clear that as the volume fraction approaches that of close packing the period cell will not have to include more than a few spheres. At intermediate volume fractions, however, the cell will have to include a lot of spheres if it is to capture the statistical properties accurately. Of course, we can use relatively small cells, repeat the calculations with different realizations of the medium and then average. In this case the question is to estimate the fluctuation of the effective coefficients from realization to realization, as a function of the period of the approximate cell.

An even more interesting aspect of numerical homogenization is the possibility of 'capturing' it directly without using the cell problem or any asymptotic analysis. That is, does there exits a numerical method that will solve the boundary value problem

$$-\nabla \cdot \left(D(\frac{\mathbf{x}}{\varepsilon}) \nabla u(\mathbf{x}) \right) = f(\mathbf{x}) \tag{4.79}$$

in a bounded region $\mathcal{O}$ with $u(\mathbf{x}) = 0$ on the boundary $\partial\mathcal{O}$ when ε is small? This question has a trivial answer when we have the computing power to resolve the oscillations in the coefficients. For example, when with a finite difference method we use a mesh whose size $h = \varepsilon/10$ then we will get good approximations. The question is interesting, however, when we consider only numerical methods with the natural complexity of the problem, that is, numerical methods that work without resolving the oscillations. This was first done by Engquist and Hou [33] for hyperbolic problems with oscillating solutions and they showed that it can be implemented with numerical grids that have random spacing comparable to ε. It is an attractive idea: if the numerical grid samples the region in an irregular way then it will capture the oscillations in the coefficients correctly without resolving them, that is, with the grid size h comparable to ε. Unfortunately attractive as the idea is it does not work for the elliptic problem (4.79) unless the coefficients are periodic [34] or the problem is one-dimensional. What is actually shown in [34] is that one particular way of implementing the random sampling idea does not work in the case of random coefficients. The general problem of capturing homogenization behavior numerically with methods of natural complexity is a very important one and progress in is likely to have profound implications in other, related areas as well.

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