

Scattering of an elastic wave from a heterogeneous material

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GENERALLY a behaviour of heterogeneous material must be described by effective material parameters depending on the propagation vector and by effective boundary conditions. Hence, most important, the wave equation must be changed in the vicinity of the boundary. These facts will be demonstrated by means of a simple scalar wave where the medium differs slightly from homogeneous one.

W ogólności, zachowanie się niejednorodnego ośrodka musi być opisane przez efektywne parametry materiałowe zależące od wektora falowego oraz przez efektywne warunki brzegowe. Oprócz tego, w pobliżu brzegu ośrodka równanie falowe musi mieć inną postać niż we wnętrzu. Te fakty będą zilustrowane na przykładzie prostej fali skalarniej, propagującej się przez ośrodek słabo-niejednorodny.

В общем случае, поведение неоднородной среды определяется эффективными параметрами материала, которые зависят от волнового вектора, и эффективными краевыми условиями. Более того, в окрестности границы волновое уравнение должно иметь другой вид, чем для толщ материала. Эти факты показаны на примере распространения скалярной волны в слабо неоднородной среде.

1. Introduction

IN ORDER to examine the problem of wave scattering from a heterogeneous material, we compare the typical length parameters. This is a question of the wave-length λ , given by the wave number k , and the length l characterizing the extension of the heterogeneities. These heterogeneities may be, for instance, inclusions or the perfect crystals comprising a polycrystal. If the relation $kl \ll 1$ holds, the material may be described by means of effective material constants calculated by a perturbation procedure [1] or by the self-consistent solution of an inclusion problem [2], or at least bounds may be given for these constants [3].

In the case $l \approx \lambda$, the reflection and transmission coefficients depend on the propagation constant k . The heterogeneous medium must be described by effective material parameters depending on k , but that does not suffice. There exists a surface layer having a thickness of order l , in which the wave equation is changed completely and the boundary conditions are quite different from the usual ones.

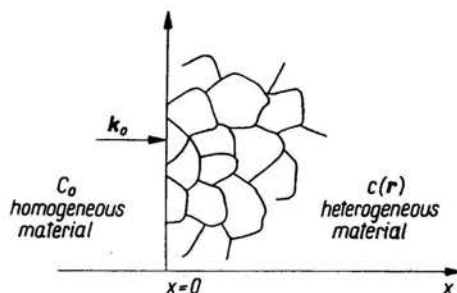
All these effects are of the same order of magnitude and they can be disregarded if, and only if, kl is sufficiently small. In order to demonstrate this fact, we use, in the interest of simplicity, a scalar model equation. It has been shown in [5, 6] that the surface layer must be taken into account in a medium with refractive index fluctuations. But media of this type effective boundary conditions present no problems; the random operator is not a differential one, as in our case (cf. Sect. 2), so that the boundary conditions for average field are of the same type as usual ones.

The propagation of scalar wave $u(\mathbf{r})$ in an inhomogeneous linear elastic medium may be governed by the Eq.

$$(1.1) \quad \rho\omega^2 u(\mathbf{r}, \omega) + \frac{\partial}{\partial \mathbf{r}} \hat{c}(\mathbf{r}) \frac{\partial}{\partial \mathbf{r}} u(\mathbf{r}, \omega) = 0,$$

where ω denotes a given frequency, ρ —constant mass density, and $\hat{c}(\mathbf{r})$ denotes a material parameter, which is a random function of positions.

We consider the reflection of a wave coming from homogeneous material at a heterogeneous semi-space with plane surface, assuming that the propagation vector \mathbf{k}_0 of the incident wave is perpendicular to the surface.



Using a tempered Heaviside function $\theta_\epsilon(x)$, the boundary conditions are implicitly contained in the wave equation (1.1) (see Sect. 2). If the fluctuations of the material parameter $c(\mathbf{r})$ are small, an ensemble average leads to an equation for the mean field:

$$(1.2) \quad \rho\omega^2 \langle u(\mathbf{r}, \omega) \rangle + \frac{\partial}{\partial \mathbf{r}} \int d\tau' c_{\text{eff}}(\mathbf{r}, \mathbf{r}') \frac{\partial}{\partial \mathbf{r}'} \langle u(\mathbf{r}', \omega) \rangle = 0.$$

This equation is of the same type as the equation of a certain model of non-local elasticity [7]. In the case where $x \gg l$, the kernel becomes dependent on the difference $\mathbf{r} - \mathbf{r}'$ if the material is statistically homogeneous; thus, for $x \gg l$ we may write

$$(1.3) \quad \rho\omega^2 \langle u(\mathbf{r}, \omega) \rangle + \frac{\partial}{\partial \mathbf{r}} \int d\tau' c_{\text{eff}}(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial \mathbf{r}'} \langle u(\mathbf{r}', \omega) \rangle = 0.$$

Now, we seek a plane-wave solution $\langle u \rangle = D_{\text{eff}} e^{i\mathbf{k}_{\text{eff}} \mathbf{r}}$ of (1.2), and obtain

$$\rho\omega^2 \langle u \rangle + \frac{\partial}{\partial \mathbf{r}} c_{\text{eff}}(\mathbf{k}_{\text{eff}}) \frac{\partial}{\partial \mathbf{r}} \langle u \rangle = 0,$$

where

$$(1.4) \quad c_{\text{eff}}(\mathbf{k}_{\text{eff}}) = \int d\tau' c_{\text{eff}}(\mathbf{r} - \mathbf{r}') e^{i\mathbf{k}_{\text{eff}}(\mathbf{r}' - \mathbf{r})}.$$

The material should be described by an effective material parameter $c_{\text{eff}}(\mathbf{k})$ depending on the propagation constant \mathbf{k} . But in the other regions, called surface layers, the integral equation (1.2) must be considered.

We compare three cases.

1. For $kl \ll 1$, the propagation of the mean field $\langle u \rangle$ behaves in the same manner as propagation in a homogeneous material $c_{\text{eff}}(0)$.

$$c_0 \quad | \quad c_{\text{eff}}(0).$$

2. Disregarding the surface layer, the material property is given by $c_{\text{eff}}(\mathbf{k})$

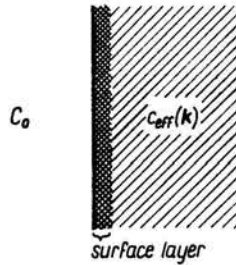
$$c_0 \quad | \quad c_{\text{eff}}(\mathbf{k}).$$

Here, the reflection and transmission-coefficient, respectively, are given by:

$$(1.5) \quad R(\mathbf{k}) = \frac{\sqrt{c_0} - \sqrt{c_{\text{eff}}(\mathbf{k})}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}(\mathbf{k})}},$$

$$(1.6) \quad D(\mathbf{k}) = \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}(\mathbf{k})}}.$$

3. Taking into account the surface layer, we have two homogeneous materials with



the parameters c_0 and $c_{\text{eff}}(\mathbf{k})$, respectively. These materials are connected by a layer in which occurs the change of the behaviour of the materials.

The coefficients $R_{\text{eff}}(\mathbf{k})$ and $D_{\text{eff}}(\mathbf{k})$ will be discussed for the special cases

a) $c_0 = \langle c \rangle,$

b) $c_0 \ll \langle c \rangle.$

We apply this restriction because in these cases, the given Fourier transform of the Green functions occurring can be easily transformed into the physical space.

2. Derivation of the effective equation

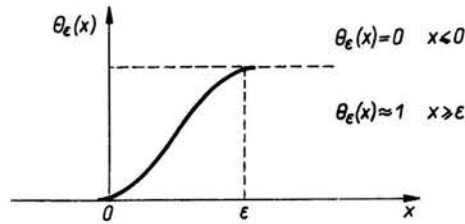
The wave u is the solution of the Eq. (1.1), which can be rewritten in the form:

$$Lu = 0,$$

where

$$(2.1) \quad L = \rho\omega^2 + \frac{\partial}{\partial \mathbf{r}} \tilde{c}(\mathbf{r}) \frac{\partial}{\partial \mathbf{r}} \quad \text{and} \quad \tilde{c}(\mathbf{r}) = c_0 + (c(\mathbf{r}) - c_0)\theta_s(x).$$

The function $\theta_\varepsilon(x)$ is a tempered Heaviside function:



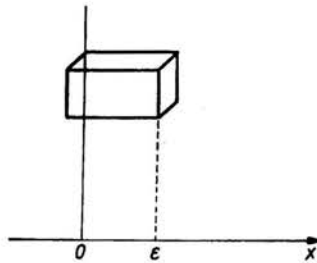
In the range $0 \leq x \leq \varepsilon$, $\theta_\varepsilon(x)$ is an arbitrary function of class C^1 . The parameter ε is very small compared with the extension of the heterogeneities

$$\varepsilon \ll l,$$

so that terms ε/l or $k\varepsilon$ can be disregarded. Then, examination of (2.1) shows:

$$(2.2) \quad u(x=0, y, z) = u(x=\varepsilon, y, z)$$

and integrating Eq. (2.1) over a small volume



we obtain, disregarding terms of the order ε

$$(2.3) \quad c_0 \frac{\partial}{\partial x} u(x, y, z) \Big|_{x=0} = c(\mathbf{r}) \frac{\partial}{\partial x} u(x, y, z) \Big|_{x=\varepsilon}.$$

In usual notations the boundary conditions are:

$$(2.4) \quad \begin{aligned} u(x=-0, y, z) &= u(x=+0, y, z), \\ c_0 \frac{\partial}{\partial x} u(x, y, z) \Big|_{x=-0} &= c(\mathbf{r}) \frac{\partial}{\partial x} u(x, y, z) \Big|_{x=+0}. \end{aligned}$$

In order to derive the effective equation, the operator L is split into two parts

$$(2.5) \quad L = \langle L \rangle + L',$$

the averaged operator $\langle L \rangle$ and the fluctuating part

$$(2.6) \quad L' = \frac{\partial}{\partial \mathbf{r}} (c(\mathbf{r}) - \langle c \rangle) \theta_\varepsilon(x) \frac{\partial}{\partial \mathbf{r}} \quad \text{with} \quad \langle L' \rangle = 0.$$

Thus the wave equation is:

$$(2.7) \quad \langle L \rangle u = \langle L \rangle \langle u \rangle - (L'u - \langle L'u \rangle).$$

By means of the averaging operator M

$$ML'u = \langle L'u \rangle,$$

we have:

$$(2.8) \quad \langle L \rangle u = \langle L \rangle \langle u \rangle - (1-M)L'u.$$

Now, a Green's function $g(\mathbf{r}, \mathbf{r}')$ is used which is defined by

$$(2.9) \quad \langle L \rangle g(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}').$$

Here δ is the Dirac delta function. The homogeneous solution must be so chosen that for $x < 0$ and $x > x'$, g describes outgoing waves only. When $c_0 = \langle c \rangle$, the solution of (2.9) is [1]:

$$(2.10) \quad g(\mathbf{r}, \mathbf{r}') = g(|\mathbf{r}-\mathbf{r}'|) = -\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi\langle c \rangle|\mathbf{r}-\mathbf{r}'|}.$$

Here, the propagation constant is

$$k = \sqrt{\frac{\rho}{c_0}} \omega = \sqrt{\frac{\rho}{\langle c \rangle}} \omega.$$

The formal solution of (2.8) now reads

$$(2.11) \quad u = (1+g*(1-M)L')^{-1}\langle u \rangle.$$

Our aim is to find an equation for $\langle u \rangle$

$$(2.12) \quad L_{\text{eff}}\langle u \rangle = 0.$$

Application of L to both sides of (2.11) yields together with (2.1):

$$(2.13) \quad Lu = L(1+g*(1-M)L')^{-1}\langle u \rangle = 0.$$

Taking the expected value of (2.13), we obtain

$$(2.14) \quad L_{\text{eff}} = \langle L(1+g*(1-M)L')^{-1} \rangle.$$

When $\langle L' \rangle = 0$ is used from (2.6) and $0(L'^3)$ is omitted, (2.14) becomes:

$$(2.15) \quad L_{\text{eff}} = \langle L \rangle - \langle L'g*L' \rangle.$$

Substituting (2.15) into (2.12) and rewriting all terms explicitly yields our main equation for $\langle u \rangle$

$$(2.16) \quad \rho\omega^2\langle u \rangle + \frac{\partial}{\partial \mathbf{r}} (c_0 + (\langle c \rangle - c_0)\theta_\varepsilon(x)) \frac{\partial}{\partial \mathbf{r}} \langle u \rangle - \frac{\partial}{\partial \mathbf{r}} \theta_\varepsilon(x) \int d\tau' \left(\frac{\partial}{\partial \mathbf{r}} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial \mathbf{r}'} \theta_\varepsilon(x') \langle (c(\mathbf{r}) - \langle c \rangle)(c(\mathbf{r}') - \langle c \rangle) \rangle \frac{\partial}{\partial \mathbf{r}'} \langle u \rangle = 0.$$

This procedure is quite general [1].

In order to simplify (2.16), it will be convenient to introduce the correlation function $K(\mathbf{r}-\mathbf{r}')$, defined by

$$(2.17) \quad \langle c \rangle^2 \alpha K(\mathbf{r}-\mathbf{r}') = \langle (c(\mathbf{r}) - \langle c \rangle)(c(\mathbf{r}') - \langle c \rangle) \rangle$$

with the small parameter

$$(2.18) \quad \alpha = \frac{\langle (c(\mathbf{r}) - \langle c \rangle) (c(\mathbf{r}) - \langle c \rangle) \rangle}{\langle c \rangle^2}.$$

Because of the statistical homogeneity assumed, the correlation function depends only on the distance $\mathbf{r} - \mathbf{r}'$, and α does not depend on \mathbf{r} . For explicit calculations, the simple correlation function $K(\mathbf{r} - \mathbf{r}') = K(|\mathbf{r} - \mathbf{r}'|) = \exp\left(-\frac{|\mathbf{r} - \mathbf{r}'|}{l}\right)$ is assumed to have the length l characterizing the extension of the heterogeneities. In what follows, we specify our considerations to a mean wave depending on x only. Thus (2.16) goes over to

$$(2.19) \quad \begin{aligned} & \rho \omega^2 \langle u \rangle + \frac{\partial}{\partial x} (c_0 + (\langle c \rangle - c_0) \theta_e(x)) \frac{\partial}{\partial x} \langle u \rangle, \\ & - \alpha \frac{\partial}{\partial x} \langle c \rangle^2 \theta_e(x) \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} \theta_e(x') K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} \langle u \rangle = 0. \end{aligned}$$

The fact that (2.19) is an equation for a field $\langle u \rangle$ in a medium with a boundary is recognized by $\theta_e(x)$, and in general also, by $g(\mathbf{r}, \mathbf{r}')$.

Now we shall seek the solution of (2.19) far from the boundary in the interior of the right half space. Here, the Green's function is given by (2.10), and we have to put $\theta_e(x) = 1$, together with $\theta_e(x') = 1$, in view of the rapid decrease of the correlation function. Then for large x , (2.19) becomes

$$(2.20) \quad g \omega^2 \langle u \rangle + \frac{\partial}{\partial x} \langle c \rangle \frac{\partial}{\partial x} \langle u \rangle - \alpha \frac{\partial}{\partial x} \langle c \rangle^2 \int d\tau' \left(\frac{\partial}{\partial x} g(|\mathbf{r} - \mathbf{r}'|) \right) \frac{\partial}{\partial x'} K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} \langle u \rangle = 0.$$

The asymptotic solution is a plane wave:

$$(2.21) \quad \langle u \rangle = D_{\text{eff}} e^{ik_{\text{eff}}x}.$$

Substituting (2.21) into (2.20) yields the following equation for the propagation constant k_{eff}

$$(2.22) \quad \rho \omega^2 - \langle c \rangle k_{\text{eff}}^2 + \alpha k_{\text{eff}}^2 \langle c \rangle^2 \int d\tau' \left(\frac{\partial}{\partial x} g(|\mathbf{r} - \mathbf{r}'|) \right) \frac{\partial}{\partial x'} K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} e^{ik_{\text{eff}}(x' - x)} = 0.$$

Let us introduce the abbreviation

$$(2.23) \quad \langle c \rangle \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} \theta_e(x') K(\mathbf{r} - \mathbf{r}') e^{ik_r(x' - x)} = J(x),$$

with $k_r = \sqrt{\frac{\rho}{\langle c \rangle}} \omega$.

We disregard terms of the order α^2 , which is consistent with omitting terms of order $O(L^3)$. From (2.22) and (2.23) we find:

$$(2.24) \quad k_{\text{eff}} = k_r \left(1 + \frac{\alpha}{2} J(\infty) \right).$$

This effective propagation constant reveals an attenuation of the wave together with an alteration in phase velocity, the discussion of these effects is given in Sect. 5. The effective material property $c_{\text{eff}}(\mathbf{k})$, defined in (1.4), is given by

$$(2.25) \quad c_{\text{eff}}(\mathbf{k}) = c_{\text{eff}}(k_r) = \langle c \rangle (1 - \alpha J(\infty)).$$

Taking into account the asymptotic behaviour of $\langle u \rangle$, let us use the comprehensive expression:

$$(2.26) \quad \langle u \rangle = \begin{cases} e^{ik_l x} + e^{-ik_l x} R_{\text{eff}}, & x < 0, \\ D_{\text{eff}} e^{ik_{\text{eff}} x} + \alpha \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} v(x), & x > 0, \end{cases}$$

$$\text{with } k_l = \sqrt{\frac{\rho}{c_0}} \omega.$$

Here, the plane wave is corrected by a new wave $v(x)$ caused by the kernel of (2.19). This kernel is not translation invariant near the boundary. The additional term is proportional to the small parameter α , since for $\alpha \rightarrow 0$ Eq. (2.19) becomes an usual propagation equation for two homogeneous media.

We decide on the assumption that $v(x)$ satisfies the condition

$$(2.27) \quad \lim_{x \rightarrow \infty} e^{-ik_{\text{eff}} x} v(x) = 0,$$

in order to decompose $\langle u \rangle$ in a well defined manner for $x > 0$. The factor

$\alpha \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}}$ appears in the definition of the additional field, in order to render more facile the equations which follow. For the same reason, the following decompositions are introduced:

$$(2.28) \quad D_{\text{eff}} = \left(\frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}}} \right)_{f.o.} + \alpha \left(\frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \right) D',$$

$$(2.29) \quad R_{\text{eff}} = \left(\frac{\sqrt{c_0} - \sqrt{c_{\text{eff}}}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}}} \right)_{f.o.} + \alpha \left(\frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \right) R'.$$

The notation $()_{f.o.}$ indicates that the usual reflexion and transmission coefficients (1.5) and (1.6) should be taken up to first order in α . From (2.25), we find that the relations

$$(2.30) \quad D(k_r) = \left(\frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}}} \right)_{f.o.} = \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \left(1 + \frac{\sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \frac{\alpha}{2} J(\infty) \right),$$

$$(2.31) \quad R(k_r) = \left(\frac{\sqrt{c_0} - \sqrt{c_{\text{eff}}}}{\sqrt{c_0} + \sqrt{c_{\text{eff}}}} \right)_{f.o.} = \frac{\sqrt{c_0} - \sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} + \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \frac{\sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \frac{\alpha}{2} J(\infty)$$

hold.

The correction terms in (2.28) to (2.31) vanish if there are two homogeneous semi-spaces with the material property c_0 and $\langle c \rangle$ respectively, since in these cases α tends to zero.

We have to omit the terms $O(\alpha^2)$ with respect to secular terms in all expressions. This means that, for instance, the plane wave (2.21) cannot be expanded into a power series of α , because x is not restricted to small values. But substituting (2.26) and (2.28) into (2.19), the term which involves the integral becomes

$$(2.32) \quad \langle c \rangle \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} \theta_\varepsilon(x') K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} e^{ik_{\text{eff}}x'} \\ = e^{ik_{\text{eff}}x} \langle c \rangle \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} \theta_\varepsilon(x') K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} e^{ik_{\text{eff}}(x' - x)}.$$

Here $e^{ik_{\text{eff}}(x' - x)}$ is multiplied by the rapidly decreasing function $K(\mathbf{r} - \mathbf{r}')$. For this reason, the difference $|x' - x|$ may be regarded as being at most of the order l ; thus

$$(2.33) \quad e^{ik_{\text{eff}}x} \langle c \rangle \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} \theta_\varepsilon(x') K(\mathbf{r} - \mathbf{r}') \frac{\partial}{\partial x'} \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} e^{ik_r(x' - x)}.$$

Using the definition (2.23), the integral part simplifies to

$$(2.34) \quad \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} e^{ik_{\text{eff}}x} ik_r J(x),$$

and the effective equation (2.19) reduces to:

(2.35)

$$\rho\omega^2 \langle u \rangle + \frac{d}{dx} (c_0 + (\langle c \rangle - c_0) - \theta_\varepsilon(x)) \frac{d}{dx} \langle u \rangle - \alpha \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \langle c \rangle \frac{d}{dx} \theta_\varepsilon(x) e^{ik_{\text{eff}}x} ik_r J(x) = 0$$

This is the equation which we shall now solve.

3. Effective boundary conditions

In view of $\varepsilon \ll l$, the first condition to be fulfilled is the continuity of the wave $\langle u \rangle$ at the boundary

$$(3.1) \quad \langle u \rangle|_{x=-0} = \langle u \rangle|_{x=0}.$$

Integration of (2.35) from zero to ε , and disregarding terms of order ε , yields

$$(3.2) \quad c_0 \frac{d}{dx} \langle u \rangle \Big|_{x=0} = \langle c \rangle \frac{d}{dx} \langle u \rangle \Big|_{x=0} - \alpha \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} ik_r \langle c \rangle (\theta_\varepsilon(\varepsilon) J(\varepsilon) - \theta_\varepsilon(0) J(0))$$

here, for continuity we put $J(\varepsilon) = J(0)$. From the definition of the tempered Heaviside function, it follows that $\theta_\varepsilon(0) = 0$ and $\theta_\varepsilon(\varepsilon) = 1$; thus, in usual notation, we have

$$(3.3) \quad c_0 \frac{d}{dx} \langle u \rangle \Big|_{x=-0} = \langle c \rangle \frac{d}{dx} \langle u \rangle \Big|_{x=+0} - \alpha \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} ik_r \langle c \rangle J(0).$$

Substituting (2.26) and (2.28)–(2.31) into the boundary conditions (3.1) and (3.3) yields

$$(3.4) \quad R' = D' + v(0)$$

and

$$(3.5) \quad D' = -\frac{\sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \left(\sqrt{\frac{c_0}{\langle c \rangle}} v(0) + \frac{1}{ik_r} v'(0) + J(\infty) - J(0) \right).$$

In (3.5), $v'(0)$ denotes the derivative of v with respect to x at the point $x = 0$. From (3.4) and (3.5), we find the effective reflection and transmission coefficients (2.28) and (2.29) to be

$$(3.6) \quad D_{\text{eff}} = \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} + \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \alpha \frac{\sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \left\{ \frac{1}{2} J(\infty) - \left[\sqrt{\frac{c_0}{\langle c \rangle}} v(0) + \frac{1}{ik_r} v'(0) + J(\infty) - J(0) \right] \right\},$$

$$(3.7) \quad R_{\text{eff}} = \frac{\sqrt{c_0} - \sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} + \frac{2\sqrt{c_0}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \alpha \frac{\sqrt{\langle c \rangle}}{\sqrt{c_0} + \sqrt{\langle c \rangle}} \left\{ \frac{1}{2} J(\infty) + \left[v(0) - \frac{1}{ik_r} v'(0) - J(\infty) + J(0) \right] \right\}.$$

Here, $v(0)$ and $v'(0)$ are not known previously and will be calculated in the next section.

In (3.6) and (3.7), and in accordance with (2.30) and (2.31) respectively, there occurs $\frac{1}{2} J(\infty)$. In the brackets, we find the correction caused by the surface layer. The expression $\frac{1}{2} J(\infty)$, and the brackets are multiplied by the same factor. This fact has a consequence concerning measurement of R_{eff} or D_{eff} , varying the parameter c_0 . Such measurements do not lead to decomposition between the influence of $c_{\text{eff}}(k)$ and that of the surface layer.

If $c_0 = \langle c \rangle$, we have, instead of (3.6) and (3.7):

$$(3.8) \quad D_{\text{eff}} = 1 + \frac{\alpha}{2} \left\{ \frac{1}{2} J(\infty) - \left[v(0) + \frac{1}{ik_r} v'(0) + J(\infty) - J(0) \right] \right\}_{c_0 = \langle c \rangle},$$

$$(3.9) \quad R_{\text{eff}} = \frac{\alpha}{2} \left\{ \frac{1}{2} J(\infty) + \left[v(0) - \frac{1}{ik_r} v'(0) - J(\infty) + J(0) \right] \right\}_{c_0 = \langle c \rangle}.$$

Within the limit $c_0 \ll \langle c \rangle$, we obtain:

$$(3.10) \quad D_{\text{eff}} = 2 \sqrt{\frac{c_0}{\langle c \rangle}} \left\{ 1 + \frac{\alpha}{2} J(\infty) - \alpha \left[\frac{1}{ik_r} v'(0) + J(\infty) - J(0) \right] \right\}_{\text{as}},$$

$$(3.11) \quad R_{\text{eff}} = -1 + 2 \sqrt{\frac{c_0}{\langle c \rangle}} \left\{ 1 + \frac{\alpha}{2} J(\infty) + \alpha \left[v(0) - \frac{1}{ik_r} v'(0) - J(\infty) + J(0) \right] \right\}_{\text{as}}.$$

Here, the notation as indicates that for the terms in brackets the asymptotic values are to be taken.

4. The solution in the surface layer

In order to determine the values $v(0)$ and $v'(0)$ in (3.6)–(3.11), we shall insert (2.26) into (2.35). With (2.22) and (2.23), the result reads

$$(4.1) \quad k_{\text{eff}}^2 v(x) + \frac{d^2}{dx^2} v(x) + \frac{d}{dx} i k_r e^{i k_{\text{eff}} x} (J(\infty) - J(x)) = 0.$$

In view of secular terms, we do not replace k_{eff} by k_r . The solution of (4.1) for $x > 0$ turns out to be

$$(4.2) \quad v(x) = \frac{1}{2} \int_x^\infty dx' e^{i k_{\text{eff}}(x-x')} \frac{d}{dx'} e^{i k_{\text{eff}} x'} (J(\infty) - J(x')) \\ - \frac{1}{2} \int_x^\infty dx' e^{i k_{\text{eff}}(x'-x)} \frac{d}{dx'} e^{i k_{\text{eff}} x'} (J(\infty) - J(x')).$$

Differentiating both sides of (4.2) twice with respect to x shows that (4.1) is fulfilled.

In order to examine the asymptotic condition (2.27), we look for the asymptotic behaviour of $J(x) - J(\infty)$. To this end, we define

$$(4.3) \quad f(x, x') = -\langle c \rangle \int dy' dz' \left(\frac{\partial^2}{\partial x \partial x'} g(\mathbf{r}, \mathbf{r}') \right) K(\mathbf{r} - \mathbf{r}'),$$

so that (2.23) becomes, omitting terms $O(\epsilon)$,

$$(4.4) \quad J(x) = \int_0^\infty dx' f(x, x') e^{i k_r (x'-x)}.$$

The expression $\frac{\partial^2}{\partial x \partial x'} g(\mathbf{r}, \mathbf{r}')$ is not a function, but a distribution [4]. It is defined in principle by

$$(4.5) \quad \int d\tau' \left(\frac{\partial^2}{\partial x \partial x'} g(\mathbf{r}, \mathbf{r}') \right) h(\mathbf{r}') = - \int d\tau' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}') \right) \frac{\partial}{\partial x'} h(\mathbf{r}').$$

We shall treat it with considerable care. First, let us consider the case $c_0 = \langle c \rangle$. Then $g(\mathbf{r}, \mathbf{r}')$ is given by (2.10) and $f(x, x') = f_\infty(x-x')$ is valid.

In order to make use of (4.5), we rewrite (4.3) with the Dirac δ -function in the form

$$(4.6) \quad f_\infty(x-x') = -\langle c \rangle \int d\tau'' \left(\frac{\partial^2}{\partial x \partial x''} g(\mathbf{r}, \mathbf{r}'') \right) K(\mathbf{r} - \mathbf{r}'') \delta(x' - x''),$$

which goes over to

$$(4.7) \quad f_\infty(x-x') = \langle c \rangle \int d\tau'' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}'') \right) \left(\frac{\partial}{\partial x''} K(\mathbf{r} - \mathbf{r}'') \right) \delta(x' - x'') \\ + \langle c \rangle \int d\tau'' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}'') \right) K(\mathbf{r} - \mathbf{r}'') \frac{\partial}{\partial x''} \delta(x' - x'').$$

The evaluation of the integrals

$$(4.8) \quad \int dy'' \int dz'' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}'') \right) \left(\frac{\partial}{\partial x''} K(\mathbf{r} - \mathbf{r}'') \right)$$

and

$$(4.9) \quad \int dy'' \int dz'' \left(\frac{\partial}{\partial x} g(\mathbf{r}, \mathbf{r}'') \right) K(\mathbf{r} - \mathbf{r}'')$$

is performed by means of the substitution

$$(4.10) \quad \begin{aligned} y - y'' &= \varrho \cos \varphi, \\ z - z'' &= \varrho \sin \varphi, \end{aligned}$$

and after the integration with respect to φ we put

$$(4.11) \quad r = \sqrt{\varrho^2 + (x - x')^2}$$

and integrate, if possible, or transform the integrals to

$$\int_{|x-x'|}^{\infty} dr \frac{e^{(ik - \frac{1}{l})r}}{r}.$$

Finally, integration with respect to x'' yields:

$$(4.12) \quad f_{\infty}(x - x') = \delta(x - x') + \frac{1}{4l} \left\{ \left[1 + 2ikl - \frac{|x - x'|}{l} (1 + ikl) \right] e^{(ik - \frac{1}{l})|x - x'|} + \left[\frac{(x - x')^2}{l^2} (1 - (ikl)^2) - 2 \right] \int_{|x - x'|}^{\infty} dr \frac{e^{(ik - \frac{1}{l})r}}{r} \right\}.$$

For large distance $|x - x'|$, the function $f(x - x')$ behaves as $\exp\left(-\frac{|x - x'|}{l}\right)$. The dominant terms for $x \approx x'$, are the δ -function and the integral with its logarithmic singularity.

The difference $J(\infty) - J(x')$ in (4.2) is proportional to $\exp\left(-\frac{x'}{l}\right)$ for large x' , so that $v(x)$ given in (4.2) fulfils the asymptotic condition (2.27). Because of the exponential decrease as $\exp\left(-\frac{x'}{l}\right)$, secular terms do not appear, if we expand $v(x)$ into a power series with respect to α such that, omitting $O(\alpha^2)$, (4.2) takes the form

$$(4.13) \quad v(x) = \frac{1}{2} \int_x^{\infty} dx' e^{ikr(x-x')} \frac{d}{dx'} e^{ikr x'} (J(\infty) - J(x')) - \frac{1}{2} \int_x^{\infty} dx' e^{ikr(x-x')} \frac{d}{dx'} e^{ikr x'} (J(\infty) - J(x')).$$

In the general case, $g(\mathbf{r}, \mathbf{r}') = g(x, x', y - y', z - z')$, we find an expression for the Green function by means of the Fourier transform with respect to $y - y'$ and $z - z'$

$$(4.14) \quad g(x, x', y, z) = \frac{1}{(2\pi)^2} \int dk_y dk_z e^{-ik_y y} e^{-ik_z z} \hat{g}(x, x', k_y, k_z).$$

With this, and with (2.1), the relation (2.9) takes the form

$$(4.15) \quad \rho\omega^2\hat{g} - [c_0 + (\langle c \rangle - c_0)\theta_s(x)](k_y^2 + k_z^2)\hat{g} + \frac{\partial}{\partial x}(c_0 + (\langle c \rangle - c_0)\theta_s(x))\frac{\partial}{\partial x}\hat{g} = \delta(x-x').$$

We observe that this equation yields boundary conditions similar to (2.4)

$$(4.16) \quad \hat{g}(-0, x', k_y, k_z) = \hat{g}(+0, x', k_y, k_z),$$

$$(4.17) \quad c_0 \frac{\partial \hat{g}}{\partial x} \Big|_{x=0} = \langle c \rangle \frac{\partial \hat{g}}{\partial x} \Big|_{x=+0}$$

Since we need $g(x, x', y, z)$ for $x' > 0$, the solution of (4.15) fulfilling the boundary conditions (4.16) and (4.17) proves to be:

$$(4.18) \quad \hat{g}(x, x', k_y, k_z) = \begin{cases} \frac{e^{ik_r^*|x-x'|} + \langle c \rangle k_r^* - c_0 k_l^*}{2ik_r^* \langle c \rangle} \frac{e^{ik_r^*(x+x')}}{2ik_r^* \langle c \rangle}, & x > 0, \\ \frac{2\langle c \rangle k_r^*}{c_0 k_l^* + \langle c \rangle k_r^*} \frac{e^{ik_r^*x} e^{-ik_l^*x}}{2ik_r^* \langle c \rangle}, & x < 0. \end{cases}$$

Here

$$k_l^* = \sqrt{k_l^2 - k_y^2 - k_z^2} \quad \text{and} \quad k_r^* = \sqrt{k_r^2 - k_y^2 - k_z^2},$$

where the real and imaginary parts of k_l^* and k_r^* are not negative for all k_y and k_z .

The first term for $x > 0$ in (4.18) leads to (2.10); the second cannot be transformed in a simple manner, but in the case $c_0 \ll \langle c \rangle$ its transformation into the physical space behaves like

$$(4.19) \quad \delta g = - \frac{e^{ik_r \sqrt{(x+x')^2 + (y-y')^2 + (z+z')^2}}}{4\pi \langle c \rangle \sqrt{(x+x')^2 + (y-y')^2 + (z-z')^2}},$$

or like (2.10), replacing there, however, $x-x'$ by $x+x'$. The correction δg is a function without any singularity in the range $x > 0$ and $x' > 0$. Therefore, the second derivative in (4.3) is a function not a distribution. From (4.3) and (4.4) it follows that

$$(4.20) \quad J(x) = \int dx' f_\infty(x-x')\theta_s(x')e^{ik_r(x'-x)} - \langle c \rangle \int d\mathbf{r}' \left(\frac{\partial^2}{\partial x'^2} \delta g(x+x', y-y', z-z') \right) K(\mathbf{r}-\mathbf{r}')\theta_s(x')e^{ik_r(x'-x)}.$$

After substituting $\mathbf{r}' - \mathbf{r} = \mathbf{r}''$ with $\frac{d}{dx''} = \frac{1}{2} \frac{d}{dx}$, the correction term may be written in the form

$$(4.21) \quad - \frac{\langle c \rangle}{4} \int_{-x}^{\infty} dx'' \int_{-\infty}^{\infty} dy'' \int_{-\infty}^{\infty} dz'' \left(\frac{\partial^2}{\partial x''^2} \delta g(2x+x'', y'', z'') \right) K(\mathbf{r}'')e^{ik_r x''}.$$

In view of $K(\mathbf{r}'') = e^{-\frac{r''}{l}}$, the values of x'' , y'' and z'' , respectively, are, at most, of the order l , so that $\frac{x''}{x}$ is very small for $x \gg l$. Now we assume $kl \approx 1$ at most; this is consistent

with application of the perturbation theory, used to arrive at (2.15) from (2.14). Then, the asymptotic value of δg may be written:

$$(4.22) \quad \delta g_{\text{as}} = -\frac{e^{ik_r(2x+x')}}{4\pi\langle c \rangle 2x}.$$

The result, after integration is that (4.20) behaves as $\frac{l}{x}$, in particular:

$$(4.23) \quad f(x, x')_{\text{as}} \sim \frac{l}{x} e^{-\frac{|x|}{l}} + f_{\infty}(x-x').$$

The surface layer is not restricted to the boundary, as in the case $c_0 = \langle c \rangle$, but its characteristic length is also l . Next we compute $v(0)$ and $v'(0)$ from (4.2):

$$(4.24) \quad v(0) = \frac{1}{2} \int_0^{\infty} dx e^{-ik_{\text{eff}}x} \frac{d}{dx} e^{ik_{\text{eff}}x} (J(\infty) - J(x)) - \frac{1}{2} \int_0^{\infty} dx e^{ik_{\text{eff}}x} \frac{d}{dx} e^{ik_{\text{eff}}x} (J(\infty) - J(x)),$$

and

$$(4.25) \quad v'(0) = \frac{ik_r}{2} \int_0^{\infty} dx e^{-ik_{\text{eff}}x} \frac{d}{dx} e^{ik_{\text{eff}}x} (J(\infty) - J(x)) \\ + \frac{ik_r}{2} \int_0^{\infty} dx e^{ik_{\text{eff}}x} \frac{d}{dx} e^{ik_{\text{eff}}x} (J(\infty) - J(x)).$$

5. Results

In exploring the example $c_0 = \langle c \rangle$, we arrived at the results (3.8), (3.9), where $v(0)$ and $v'(0)$ are given by (4.24) and (4.25), respectively. Here, $J(x)$ is defined by (4.4), with $f(x, x') = f_{\infty}(x-x')$ from (4.12) and

$$(5.1) \quad J(\infty) = \int_{-\infty}^{\infty} dx f_{\infty}(x) e^{ikx}.$$

A straightforward rearrangement yields:

$$(5.2) \quad D_{\text{eff}} = 1 + \frac{\alpha}{2} \left[\frac{1}{2} \int_{-\infty}^{\infty} dx f_{\infty}(x) e^{ikx} - ik \underbrace{\int_0^{\infty} dx x f_{\infty}(x) e^{-ikx}}_{\text{surface layer}} \right],$$

$$(5.3) \quad R_{\text{eff}} = \frac{\alpha}{2} \left[\frac{1}{2} \int_{-\infty}^{\infty} dx f_{\infty}(x) e^{ikx} + \frac{1}{2} \underbrace{\int_0^{\infty} dx f_{\infty}(x) (e^{ikx} - e^{-ikx})}_{\text{surface layer}} \right].$$

Calculation of (5.2) and (5.3) yields somewhat lengthy expressions which we shall not write out. We shall give the result up to order $(ikl)^2$. In doing this, $f(x)$ is expanded as

$$(5.4) \quad f_{\infty}(x) = \delta(x) + \frac{1}{l} f_0\left(\frac{x}{l}\right) + ikl \frac{1}{l} f_1\left(\frac{x}{l}\right) + \frac{1}{2} (ikl)^2 \frac{1}{l} f_2\left(\frac{x}{l}\right).$$

We observe that

$$(5.5) \quad f_1\left(\frac{x}{l}\right) = 0.$$

which is to be seen, without any calculation, from (4.3) with (2.10), by evaluating $g(\mathbf{r}-\mathbf{r}')$ into a power series of k . It will be convenient to introduce $\frac{x}{l} = z$. Omitting terms of $O((ikl)^3)$, the effective coefficients D_{eff} and R_{eff} become:

$$(5.6) \quad D_{\text{eff}} = 1 + \frac{\alpha}{2} \left\{ \frac{1}{2} + \int_0^{\infty} dz f_0(z) + \frac{1}{2} (ikl)^2 \int_0^{\infty} dz (f_2(z) + z^2 f_0(z)) - ikl \int_0^{\infty} dz z f_0(z) \right\},$$

$$(5.7) \quad R_{\text{eff}} = \frac{\alpha}{2} \left\{ \frac{1}{2} + \int_0^{\infty} dz f_0(z) + \frac{1}{2} (ikl)^2 \int_0^{\infty} dz (f_2(z) + z^2 f_0(z)) + ikl \int_0^{\infty} dz z f_0(z) + \frac{1}{2} (ikl)^2 \int_0^{\infty} dz f_0(z) z^2 \right\}.$$

But disregarding the surface layer, we find:

$$(5.8) \quad D = 1 + \frac{\alpha}{2} \left\{ \frac{1}{2} + \int_0^{\infty} dz f_0(z) + \frac{1}{2} (ikl)^2 \int_0^{\infty} dz (f_2(z) + f_0(z) z^2) \right\},$$

$$(5.9) \quad R = \frac{\alpha}{2} \left\{ \frac{1}{2} + \int_0^{\infty} dz f_0(z) + \frac{1}{2} (ikl)^2 \int_0^{\infty} dz (f_2(z) + f_0(z) z^2) \right\}.$$

This procedure has removed all the parameters in the integrals; their values are obtained by comparing (5.4) with (4.12):

$$(5.10) \quad \int_0^{\infty} dz f_0(z) = -\frac{1}{3}, \quad \int_0^{\infty} dz (f_2(z) + f_0(z) z^2) = -\frac{7}{15},$$

$$\int_0^{\infty} dz z f_0(z) = -\frac{1}{8}, \quad \int_0^{\infty} dz z^2 f_0(z) = -\frac{2}{15}.$$

Thus

$$(5.11) \quad D_{\text{eff}} = 1 + \frac{\alpha}{2} \left\{ \frac{1}{6} + \frac{1}{8} ikl - \frac{7}{15} \frac{1}{2} (ikl)^2 \right\},$$

$$(5.12) \quad R_{\text{eff}} = \frac{\alpha}{2} \left\{ \frac{1}{6} - \frac{1}{8} ikl - \frac{11}{15} \frac{1}{2} (ikl)^2 \right\}$$

and

$$(5.13) \quad D = 1 + \frac{\alpha}{2} \left\{ \frac{1}{6} - \frac{7}{15} \frac{1}{2} (ikl)^2 \right\},$$

$$(5.14) \quad R = \frac{\alpha}{2} \left\{ \frac{1}{6} - \frac{7}{15} \frac{1}{2} (ikl)^2 \right\}.$$

The coefficients D_{eff} and D differ one from the other in phase by an amount of the order kl while the difference in their absolute values is of order $(kl)^2$. The same applies to R_{eff} and R .

In the case $c_0 \ll \langle c \rangle$, we have terms as in (5.11) and (5.12), respectively, and additional parts resulting from δg . Nevertheless, it is also true that the alteration in the phase is proportional to kl and the difference of the absolute values has a factor $(kl)^2$. The physical importance of this result is as follows: in far as k -dependence of the reflection- and transmission-coefficients must be taken into account, it is necessary to describe heterogeneous material by the effective material parameters $c_{\text{eff}}(k)$ and by effective boundary conditions: further, the wave equation turns out to be quite different from the usual ones in the vicinity of the boundary. This is already valid in first order in kl .

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