Archives of Mechanics • Archiwum Mechaniki Stosowanej • 28, 3, pp. 325–332, Warszawa 1976

Derivation of a generalized continuum theory for heterogeneous materials

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STARTING from the microstructure of a heterogeneous (composite) material by means of ensemble-averaging a macroscopic continuum theory is derived. Besides the mean field it contains additional degrees of freedom, called "multipole"-fields. It is shown that, as a matter of principle, a local theory of that kind, described by differential equations, cannot be achieved up to an arbitrarily high accuracy. On the contrary, it is restricted to the long-wave-range. In the present paper the approach is explained in a rather general notion and illustrated by means of a simple model. Application to the elastic case is reserved to a subsequent paper.

Wychodząc z mikrostruktury materiału heterogennego (kompozytu) i wykorzystując uśrednienie zbioru wyprowadzono makroskopową teorię kontinuum. Oprócz pola uśrednionego zawiera ona dodatkowe stopnie swobody zwane "multipolami". Wykazano, że w zasadzie tego rodzaju teorii lokalnej, opisanej równaniami różniczkowymi, nie można otrzymać z dowolnie dużą dokładnością, ponieważ jest ona ograniczona do zakresu fal długich. W niniejszej pracy sposób podejścia wyjaśniono ogólnie i zilustrowano prostym modelem. Zastosowanie niniejszej teorii do przypadku sprężystego będzie przedmiotem następnej pracy.

Исходя из микроструктуры гетерогенного материала (композита) и используя усреднение множества, выведена макроскопическая теория континуум. Кроме усредненного поля содержит она дополнительные степени свободы, называемые „мультиполями''. Показано, что в принципе этого рода локальной теории, описанной дифференциальными уравнениями, не можно получить с произвольно большой точностью. Напротив она ограничена диапазоном длинных волн. В настоящей работе способ подхода объяснен общим образом и иллюстрирован простой моделью. Применение настоящей теории к упругому случаю будет предметом следующей работы.

Introduction

MANY continuum theories have been proposed which are generalized in the sense that, besides the mean displacement field, additional degrees of freedom are assumed (micromorphic, micropolar, multipolar theories) [1, 2, 3]. The aim is to characterize the internal structure of the body in more detail. Especially, in some cases this approach has been used for describing heterogeneous materials, for instance laminated or fibre-reinforced bodies [4, 5, 6]. Apart from such well established applications, there seems to be a lack concerning a sufficient physical interpretation of the additional degrees of freedom. In the same way, physical reasons for the accepted constitutive relations are desirable.

This state of affairs suggests an attempt of deriving such a generalized continuum theory by means of remodeling and averaging the exact microscopic equations. The notation "microscopic" does not refer to the atomic scale but to the characteristic length of heterogeneity. Obviously, in our case it is sufficient to explore the general structure of the macroscopic equations without taking care of numerical coefficients. The latter will

strongly depend on the underlying special model whereas the form of the field equations is expected to posses a more general validity.

In the first section a scheme is offered according to which such a transition from the microscopic equations to macroscopic ones may be performed. This scheme is restricted to linear phenomena like elasticity, conductivity et al.

In the second section the general considerations of the first one are briefly illustrated by means of a simple model. The more complicated but most interesting case of elasticity will be treated in a subsequent paper.

1. The general scheme

We consider inclusions E being stochastically distributed within a matrix M. In M a certain field $u(r, t)$ may be governed by a field equation

$$L_M u = f, \tag{1.1}$$

where L_M is a linear differential operator with constant coefficients, f being a source term. In the same way, inside the i-th inclusion we have

$$L_E^i u = f, \tag{1.2}$$

L_E^i being of the same type as L_M.

At an arbitrary point an equation

$$Lu = \left\{L_M + \sum_i L^i\right\} u = f \tag{1.3}$$

holds. Concerning time dependence le tus think of a Fourier-transformation to be carried out, such that a frequency ω will appear. In Eq. (1.3) L is a *stochastic* operator with coefficients being piecemeal constant, and

$$L^i = \begin{cases} L_E^i - L_M & \text{inside the } i\text{-th inclusion,} \\ 0 & \text{otherwise.} \end{cases} \tag{1.4}$$

The final aim is the replacement of the microscopic field equation (1.3) by a macroscopic one for the mean field $\langle u \rangle$, supplemented by field equations for additional degrees of freedom. The symbol $\langle \ldots \rangle$ denotes the average over an ensemble of samples, being macroscopically equivalent but differing from one another microscopically by various arrangements of the inclusions. The additional degrees of freedom are related to the fluctuations of the field $u(r, t)$.

Let us write the general solution of Eq. (1.2) as

$$u = (L_E^i)^{-1} f + \sum_\alpha \varphi_\alpha^i Q_\alpha^i, \tag{1.5}$$

where the first term denotes the particular solution vanishing on the surface of the i-th inclusion. The second term is a solution of the homogeneous equation expressed by an appropriate system φ_α^i, being complete on the surface of the i-th inclusion.

The coefficients Q_α^i, whose values are beforehand open, denote the degrees of freedom

within the i-th inclusion. Generalizing simple cases, henceforth they should be called "multipoles".

Now, the Eq. (1.3) is formally remodeled into an integral equation

$$u = L_M^{-1}\Big\{f - \sum_i L^i u\Big\}, \tag{1.6}$$

where L_M^{-1} is that Green-operator of the infinite homogeneous matrix whose kernel vanishes at infinity. Inserting (1.5) into (1.6) yields

$$u = L_M^{-1}\Big\{f - \sum_i \Big[(L_E^i)^{-1} f + \sum_\alpha \varphi_\alpha^i Q_\alpha^i\Big]\Big\}. \tag{1.7}$$

Here we have taken into account that, according to the Eq. (1.4), on the right-hand side of the Eq. (1.6) there appears only the u-field in the interior of the i-th inclusion.

The Eq. (1.7) shows us, that the microscopic problem is reduced to the task of finding the multipoles Q_α^i. Equations for these quantities can be obtained from the Eqs. (1.7) and (1.5). To this end, we apply the operator L^j to the Eq. (1.7), taking into account again, that, because of (1.4) the field-variable u occuring behind L^j can be replaced by the Eq. (1.5). Thus, we obtain

$$L^j\Big\{(L_E^j)^{-1} f + \sum_\alpha \varphi_\alpha^j Q_\alpha^j\Big\} = L^j L_M^{-1}\Big\{f - \sum_i L^i\Big[(L_E^i)^{-1} f + \sum_\alpha \varphi_\alpha^i Q_\alpha^i\Big]\Big\}. \tag{1.8}$$

It is suitable to introduce a system of functions $\bar{\varphi}_\alpha^i$ being adjoint to φ_α^i in the sense that

$$\int dV \bar{\varphi}_\alpha^i L^i (1 + L_M^{-1} L^i) \varphi_\beta^i = \delta_{\alpha\beta}. \tag{1.9}$$

Such a system can be obtained, for instance, from

$$\begin{aligned} \sum_\beta \varepsilon_{\alpha\beta}^i \varphi_\beta^i &= (\varphi_\alpha^i)^*, \\ \varepsilon_{\alpha\beta}^i &= \int dV (\varphi_\alpha^i)^* L^i (1 + L_M^{-1} L^i) \varphi_\alpha^i. \end{aligned} \tag{1.10}$$

We get a system of equations for the unknown Q_α^i by means of applying the operator $\int dV \bar{\varphi}_\alpha^i$ to the Eq. (1.8).

With the aid of the abbreviations

$$\begin{aligned} \tilde{A}_{\alpha\beta}^{ij} &\equiv -\int dV \bar{\varphi}_\alpha^i L^i L_M^{-1} L^j \varphi_\beta^j, \\ \tilde{B}_\alpha^i[f] &\equiv \int dV \bar{\varphi}_\alpha^i L^i \Big\{L_M^{-1}\Big[f - \sum_j L^j (L_E^j)^{-1} f\Big] - (L_E^j)^{-1} f\Big\}, \end{aligned}$$

the result takes the compact form

$$Q_\alpha^i = \tilde{B}_\alpha^i[f] + \sum_{j(\neq i)} \sum_\beta \tilde{A}_{\alpha\beta}^{ij} Q_\beta^j. \tag{1.11}$$

Accordingly, the multipoles depend on the positions of all the inclusions, whereas L^i, φ_α^i depend on the position of the i-th inclusion only. Concerning ensemble average of Eq. (1.7), this fact gives rise to a decomposition as

$$\langle L^i \varphi_\alpha^i Q_\alpha^i \rangle = \langle L^i \varphi_\alpha^i \langle Q_\alpha^i \rangle_{\mathbf{r}^i} \rangle, \tag{1.12}$$

where $\langle \ldots \rangle_{\mathbf{r}^i}$ is the average under the condition that the i-th inclusion is situated at $\mathbf{r}^i$.

In the special case of identical inclusions (equal size and material) we consider

$$\langle Q_\alpha^i \rangle_{\mathbf{r}^i} \equiv Q_\alpha(\mathbf{r}^i) \tag{1.13}$$

as macroscopic fields, i.e. as additional degrees of freedom besides $\langle u \rangle$.

According to the Eq. (1.7) the field equation for $\langle u \rangle$ takes the form

$$L_M \langle u \rangle = \langle f \rangle - \int dV^{i1} g(\mathbf{r}^i)\, L^i (L_E^i)^{-1} \langle f \rangle_{\mathbf{r}^i} - \sum_\alpha \int dV^{i1} g(\mathbf{r}^i)\, L^i \varphi_\alpha^i Q_\alpha(\mathbf{r}^i), \tag{1.14}$$

where ${}^1g(\mathbf{r})$ denotes the one-particle distribution function.

Before we go over to the average of the Eq. (1.11) let us rewrite this equation, namely, replacing $\langle f \rangle$ within $\tilde{B}_\alpha^i[f]$ by means of the Eq. (1.14). The result is

$$Q_\alpha^i = B_\alpha^i[f] + \sum_{j(\neq i)} \sum_\beta A_{\alpha\beta}^{ij} Q_\beta^j, \tag{1.15}$$

where

$$A_{\alpha\beta}^{ij} \equiv - \int dV \bar{\varphi}_\alpha^i L^i L_M^{-1} (1 - \mathcal{M}) L^j \varphi_\beta^j,$$

$$B_\beta^i[f] \equiv \int dV \bar{\varphi}_\alpha^i L^i \Big\{ \langle u \rangle + L_M^{-1} \Big[(1 - \mathcal{M}) f - \sum_{j(\neq i)} (1 - \mathcal{M}) L^j (L_E^j)^{-1} f \Big] - (L_E^i)^{-1} f \Big\}.$$

The operator $\mathcal{M}(\ldots) \equiv \langle \ldots \rangle$ affects the average of all the terms subsequent to $\mathcal{M}$, inclusive Q_α^i which appear after $A_{\alpha\beta}^{ij}$. With it, the $A_{\alpha\beta}^{ij}$ become operators.

In order to get equations for the macroscopic field $Q_\alpha(\mathbf{r})$, the following procedure is proposed. From the Eq. (1.11) we obtain a hierarchy as

$$\begin{aligned} \langle Q \rangle &= \langle B \rangle + \langle AQ \rangle, \\ \langle AQ \rangle &= \langle AB \rangle + \langle AAQ \rangle, \\ \langle AAQ \rangle &= \langle AAB \rangle + \langle AAAQ \rangle, \\ &\ldots \end{aligned}$$

where, for the sake of clarity, all indices and sums are omitted. The brackets denote conditional averages analogous to the Eq. (1.13). Since this infinite hierarchy does not permit a direct calculation of $Q_\alpha(\mathbf{r}^i) \equiv \langle Q_\alpha^i \rangle_{\mathbf{r}^i}$, it must be closed. This may be done, for instance, replacing Q_α^i by its mean value $Q_\alpha(\mathbf{r}^i)$ in the last term of the m-th equation. Then successive substitution finally leads to equations of the type

$$\begin{aligned} Q_\alpha(\mathbf{r}) &= {}^m\mathscr{C}[\mathbf{r}, f] + \int dV' {}^m\mathscr{B}(\mathbf{r}, \mathbf{r}') \langle u(\mathbf{r}') \rangle + \sum_\beta \int dV' {}^m\mathscr{A}_{\alpha\beta}(\mathbf{r}, \mathbf{r}') Q_\beta(\mathbf{r}'), \\ L_M \langle u(\mathbf{r}) \rangle &= \mathscr{E}[\mathbf{r}, f] + \sum_\alpha \int dV' \mathscr{D}_\alpha(\mathbf{r}, \mathbf{r}') Q_\alpha(\mathbf{r}'). \end{aligned} \tag{1.16}_{1,2}$$

The last equation is identical with the Eq. (1.14). The kernel ${}^m\mathscr{A}_{\alpha\beta}$ means the conditional average for two inclusions being fixed at $\mathbf{r}$ and $\mathbf{r}'$:

$${}^m\mathscr{A}_{\alpha\beta}(\mathbf{r}, \mathbf{r}') \equiv {}^1g^{-1}(\mathbf{r}) \sum_{i_k} \sum_{\alpha_k} \langle A_{\alpha\alpha_1}^{ii_1} A_{\alpha_1\alpha_2} \ldots A_{\alpha_{m-1}\beta}^{i_{m-1}j} \rangle_{\substack{\mathbf{r}^i = \mathbf{r} \\ \mathbf{r}^j = \mathbf{r}'}}. \tag{1.17}$$

This equation shows us that ${}^m\mathscr{A}_{\alpha\beta}$ contains the distribution-function for $m+1$ inclusions. Therefore, the considered approximation disregards correlations between more than $m+1$ grains.

The Eq. (1.17) is suitably illustrated as a sum of irreducible graphs (Fig. 1).

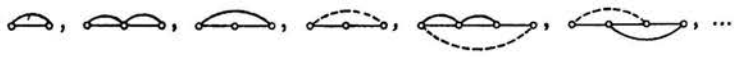

FIG. 1.

This is explained as follows: A straight line •—• means any $\tilde{A}^{ij}_{\alpha\beta}$ where the vertices (points) denote the position and the multipole-index.

In order the perform the average, the vertices have to be connected in all possible ways by correlation-functions and autocorrelation-functions. These ones are symbolized by full and dashed bows, respectively. Further, integration (summation) over the positions and multipoles of the interior vertices is prescribed. However, graphs containing autocorrelation between neighbouring vertices as well as reducible graphs are excluded. The latter are those which decay into two graphs by intersecting any $\tilde{A}^{ij}_{\alpha\beta}$-line. The restriction to irreducible graphs is caused by the operator $(1-\mathscr{M})$ in (1.15).

Obviously, our aim of writing down a finite system of differential equations has not yet been achieved. The system (1.16) consists of integral equations for the mean field $\langle u\rangle$ and an infinite number of multipoles.

In order to overcome these difficulties we decide for the following procedure. First of all, for the sake of simplicity, statistical homogeneity is assumed; that is

$$
\begin{aligned}
{}^m\mathscr{A}_{\alpha\beta}(\mathbf{r},\mathbf{r}') &\equiv {}^m\mathscr{A}_{\alpha\beta}(\mathbf{r}-\mathbf{r}'),\\
{}^m\mathscr{B}_{\alpha}(\mathbf{r},\mathbf{r}') &\equiv {}^m\mathscr{B}_{\alpha}(\mathbf{r}-\mathbf{r}'),\\
\mathscr{D}_{\alpha}(\mathbf{r},\mathbf{r}') &\equiv \mathscr{D}_{\alpha}(\mathbf{r}-\mathbf{r}').
\end{aligned}
\tag{1.18}
$$

Consequently, the Fourier-transform of (1.16) turns out to be an algebraic system

$$
\begin{aligned}
\hat{Q}_{\alpha} &= \sum_{\beta} {}^m\hat{\mathscr{A}}_{\alpha\beta}\hat{Q}_{\beta} + {}^m\hat{\mathscr{B}}_{\alpha}\langle\hat{u}\rangle + \hat{\mathscr{C}}[f],\\
\hat{L}_M\langle\hat{u}\rangle &= \sum_{\alpha} \hat{\mathscr{D}}_{\alpha}\hat{Q}_{\alpha} + \hat{\mathscr{E}}[f].
\end{aligned}
\tag{1.19}_{1,2}
$$

(The roof indicates the Fourier-transform).

Further, under the restriction to long wave-lengths, i.e. small $\mathbf{k}$, we try an expansion of the coefficients with respect to k and to the frequency ω. Truncating these series at a certain power of k and ω and retransformation into the physical space lead to a system of differential equations of corresponding order. Moreover, this approximation would permit to single out higher multipoles which contribute to the Eq. $(1.19)_2$ in an order of k which is beyond the considered accuracy such that they can be dropped altogether. In this way, finally, our system would become a finite one.

The realization of this program up to an arbitrarily high order is possible if only there is a suitable dissipative mechanism, which causes that $\mathscr{A}_{\alpha\beta}$ tends to zero more rapidly than any power of $1/r$. Otherwise we can be sure that the Green-functions behave

like $1/r$ ($r \to \infty$). It can be shown that in this case graphs will occur which decrease like a power of $1/r$ only, even when the correlation-functions are assumed to decrease exponentially for example (Fig. 2)

FIG. 2.

The Fourier-transform of these contributions cannot be expanded into a power series of k. Besides the powers there appear terms like $k^n \ln k$. Since they do not go over to differential operators by retransformation, our program is realizable only up to a restricted order. Higher accuracy can be achieved only by nonlocal continuum theories.

2. Illustration by means of a model

In the following the statements of the first section may be briefly illustrated by means of a special model. We restrict ourselves to spherical inclusions of equal size and material. Further, we consider a scalar model theory with the model-operator

$$
\begin{aligned}
L &= \varrho(\mathbf{r})\omega^2 + \nabla c(\mathbf{r})\nabla, \\
\varrho(\mathbf{r}) &= \varrho_M + (\varrho_E - \varrho_M)\Theta(R - |\mathbf{r}-\mathbf{r}^i|), \\
c(\mathbf{r}) &= c_M + (c_E - c_M)\Theta(R - |\mathbf{r}-\mathbf{r}^i|), \\
L_M &= \varrho_M\omega^2 + c_M\Delta, \\
L^i &= (\varrho_E - \varrho_M)\Theta(R - |\mathbf{r}-\mathbf{r}^i|)\omega^2 + (c_E - c_M)\nabla\Theta(R - |\mathbf{r}-\mathbf{r}^i|)\nabla.
\end{aligned} \tag{2.1}
$$

R is the radius of the inclusions, $\mathbf{r}^i$ the position vector of the i-th inclusion. Because of the spherical symmetry, the system φ^i_α (1.5) is chosen as

$$
\varphi^i_\alpha \equiv \varphi^i_{lm} = \frac{j_e(\varkappa|\mathbf{r}-\mathbf{r}_1|)}{j_e(\varkappa R)}\, Y_{lm}(\mathbf{r}-\mathbf{r}^i), \tag{2.2}
$$

where Y_{lm} denotes the spherical harmonics and

$$
j_e(z) \equiv \sqrt{\frac{\pi}{2z}}\, J_{l+\frac{1}{2}}(z)
$$

the spherical Bessel-function of the first kind. The wave-number $\varkappa$ is given by the dispersion relation of the inclusions,

$$
\varkappa = \sqrt{\frac{\varrho_E}{c_E}}\,\omega.
$$

The adjoint system $\bar{\varphi}^i_{lm}$ (1.10) is proportional to $(\varphi^i_{lm})^*$.

The execution of the program, skeched in the first section, yields the following results.

For sufficiently small wavevector k and frequency $\omega \sim \varkappa$ the leading terms in the system (1.16) behave like

$$
\begin{aligned}
&\mathscr{A}_{0000} \sim (kR)^0(\varkappa R)^2,\\
&\mathscr{A}_{00lm} \sim (kR)^l, \qquad l \neq 0,\\
&\mathscr{A}_{lm00} \sim (kR)^l(\varkappa R)^2, \qquad l \neq 0,\\
&\mathscr{A}_{lmpq} \sim (kR)^{|l-p|}, \qquad \text{otherwise},\\
&\mathscr{B}_{lm} \sim (kR)^l, \quad \mathscr{D}_{00} \sim (\varkappa R)^2, \quad \mathscr{D}_{lm} \sim (kR)^l, \quad l \neq 0.
\end{aligned} \tag{2.3}
$$

Here we have assumed that the correlation lengths are of the order of magnitude R (inclusion radius). Otherwise R has to be replaced by the largest characteristic correlation length. According to a remark in the introduction of this paper, the calculation of numerical coefficients has not been carried out. No general assertions about the inhomogeneities ${}^m\mathscr{C}$ and $\mathscr{E}$ of the Eqs. (1.16) can be made. They may assume an arbitrary order of magnitude according to the choice of the source term f. However, this does not matter since we will restrict ourselves to free waves, $f = 0$.

Besides the leading terms (2.3) there will occur additional terms with higher powers of k and ω. Moreover, as has been mentioned above, we are confronted with logarithmic terms, namely, in lowest order

$$
\begin{aligned}
&\mathscr{A}_{0000} \to (kR)^4(\varkappa R)^2\ln(kR),\\
&\mathscr{A}_{00lm} \to (kR)^{l+4}\ln(kR), \qquad l \neq 0,\\
&\mathscr{A}_{ln00} \to (kR)^{l+4}(\varkappa R)^2\ln(kR), \qquad l \neq 0,\\
&\mathscr{A}_{lmpq} \to (kR)^{l+p+4}\ln(kR) \qquad \text{otherwise},\\
&\mathscr{B}_{lm} \to (kR)^{l+6}\ln(kR),\\
&\qquad \text{or } (kR)^{l+4}(\varkappa R)^2\ln(kR).
\end{aligned} \tag{2.4}
$$

As already discussed, these terms do not correspond to any differential operator. Consequently, one can achieve a localized theory, governed by differential equations, if only these contributions are negligible. Moreover, our considerations may be restricted to the case that k and $\varkappa$ are of the same order of magnitude. In analogy to crystal vibrations we speak about "acoustic modes" in contradistinction to "optical modes", where $\varkappa \neq 0$ when $k \to 0$. The latter ones are related to vibrations of the inclusions, most of which are decoupled from the mean field $\langle u\rangle$.

In the case of acoustic branches a careful inspection of the Eqs. (1.19) shows that for small k the multipoles reveal the same order of magnitude as the coefficients $\mathscr{B}_{lm}$, i.e.

$$Q_{lm} \sim (kR)^l\langle u\rangle. \tag{2.5}$$

On the other hand, disentangling the system (1.19) step by step leads to the following conclusion: If the logarithmic terms are disregarded, then in the Eq. $(1.19)_2$ an error is caused whose order of magnitude is $(kR)^8\ln(kR)\cdot\langle u\rangle$. Therefore it is meaningless to take into regard terms of higher order than $k^7\langle u\rangle$ in the Eq. $(1.19)_2$ so far as we decide for a local approximation. This fact in connection with (2.5) and $\mathscr{D}_{lm} \sim (kR)^l$ means that all the multipoles with $l > 3$ may be neglected altogether. In this way, the approximation

which has been introduced for the sake of localization automatically reduces the infinite number of multipoles to a finite one.

This enables us to eliminate the multipoles from the system $(1.19)_{1,2}$ to obtain an equation for the mean field $\langle u \rangle$ alone. After retransformation into the physical space it is the question of a differential equation being at most of seventh order.

The relative error, which is caused by localization in the equation for mean field $\langle u \rangle$, is of the order $(kR)^6 \ln(kR)$. This can easily be seen observing that the operator L_M has the order k^2.

Summarizing we assert that the proposed procedure yields in fact local continuum theories with additional degrees of freedom. However, as a matter of principle, their validity is restricted to a certain degree of accuracy which depends on the considered wave-lengths. Higher accuracy can be achieved only by use of nonlocal theories.

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