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The Wigner potential method in the investigation of thermal properties of regular composites

S. MAY, S. TOKARZEWSKI and A. ZACHARA (WARSZAWA)

FOR PERIODIC, two-dimensional potentials satisfying the Laplace equation, a new functional basis, different from that used by RAYLEIGH [1], has been derived. This basis allowed us to construct a simple recurrence formulae for evaluation of an effective transport coefficients for regular two-dimensional composites. As an example, the power expansion of an overall conductivity for square array of circular cylinders has been evaluated.

1. Governing equations

THE TEMPERATURE distribution and the effective conductivity of composites of regular structure were first investigated by RAYLEIGH [1]. He performed calculations for rectangular arrays of circular as well as spherical inclusions. The approach of Rayleigh was next developed by many other authors [2–4]. In this paper, we present a method of solving the two-dimensional periodic problems by using a new functional basis different from that used by Rayleigh. This basis appears to be very convenient for seeking the solutions of Laplace equation and leads to very effective algorithms.

Let us consider a material composed of circular cylinders of conductivity λ_d, embedded in a matrix of conductivity λ_c. The composite is subjected to an external linear temperature field. The elementary cell is presented in Fig. 1. Let a be the cylinder radius, l – the distance between the cylinder axes, T^d and T^c – the temperature of inclusions and matrix, respectively. The temperature field in a unit cell fulfills the conductivity equations

$$\begin{aligned} \nabla^2 T^c &= 0 \qquad \text{for} \quad r > a, \\ \nabla^2 T^d &= 0 \qquad \text{for} \quad r < a, \end{aligned} \tag{1.1}$$

and the boundary conditions for $r = a$

$$\begin{aligned} T^c &= T^d, \\ \lambda_c \frac{\partial T^c}{\partial r} &= \lambda_d \frac{\partial T^d}{\partial r}, \end{aligned} \tag{1.2}$$

where r, θ are polar coordinates with the origin located on the cylinder axis.

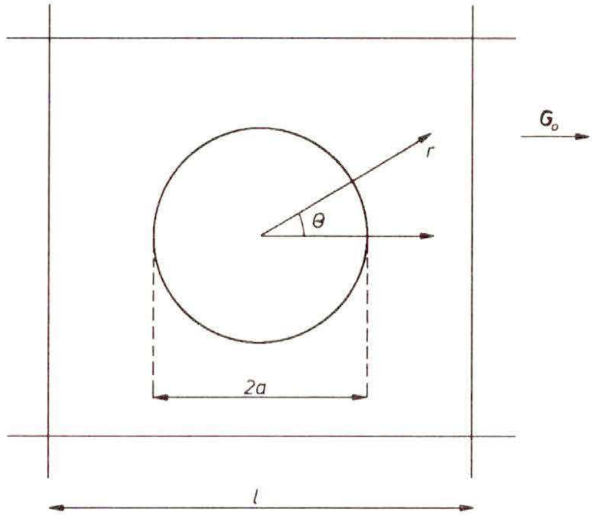

FIG. 1.

Rayleigh obtained the solution of Eqs. (1.1) in the form:

$$
\begin{aligned}
T^c(r,\theta) &= \sum_{k=1}^{\infty}\left(a_k r^k + \frac{b_k}{r^k}\right)\cos k\theta\,,\\
T^d(r,\theta) &= \sum_{k=1}^{\infty} c_k r^k \cos k\theta\,.
\end{aligned}
\tag{1.3}
$$

The solution may be interpreted as generated by an infinite system of multipoles located at the cylinder axes. We have here three infinite sets of coefficients a_k, b_k, c_k, $(k = 1, 3, \ldots)$ since, due to the symmetry conditions, only odd values of k are allowed [1]. With the aid of the boundary conditions (1.2), the coefficients a_k and c_k may be expressed as linear functions of b_k. To determine b_k, Rayleigh made an assumption that the part of the potential in the unit cell corresponding to the term of Eq. $(1.3)_1$ which is non-singular in the unit cell center $r = 0$ resulted from two sources. The first of them is the external gradient of temperature. The second one is a joint influence of the multipoles from the other cells corresponding to the terms of Eq. $(1.3)_1$ which are singular in the centers of these cells [1]. This assumption leads to the following infinite system of equations for the coefficients b_k,

$$
\delta_{k,1} + k!\,\frac{(u+2)}{ua^{2k}}b_k = \sum_{j=1}^{\infty}\frac{(k+j-1)!}{(j-1)!}S_{k+j}b_j, \qquad k = 1,3,5\ldots, \tag{1.4}
$$

where

$$
u = \frac{\lambda_d}{\lambda_c} - 1, \tag{1.5}
$$

$$S_m = \sum_{\{n\}} \frac{1}{(x_n + iy_n)^m}. \tag{1.6}$$

Symbols S_m denote the Rayleigh sums, (x_n, y_n) are Cartesian coordinates of the centers of the cells, i is an imaginary unit and $\{n\}$ denotes summation to infinity in the directions of x and y over all cylinder centers lying outside the unit cell. The sums S_m depend on the geometrical properties of the array. Numerical values of S_m for square and hexagonal arrays are given in [2].

The approximate values of b_k can be calculated from Eq. (1.4) subjected to truncation. The effective conductivity of a composite depends on the coefficient b_1 according to the formula derived by RAYLEIGH [1],

$$\mu = \frac{\lambda_{\text{cf}}}{\lambda_c} = 1 - 2\pi b_1. \tag{1.7}$$

For a square array of cylinders, the temperature distribution $T^i(r, \theta; \varphi, u)$ and the effective conductivity $\mu(\varphi, u)$ depend on two dimensionless quantities: the cylinder volume fraction φ and physical properties of the components represented by u (1.5). Coefficients a_k, b_k and c_k appearing in (1.3) are functions of φ and u.

It is well known that the Rayleigh method provides the non-unique solutions for λ_{ef}, since the second Rayleigh's sum S_2 over the infinite array of cylinders is only conditionally convergent, i.e., it depends on the shape of the exterior boundary of the composite. This was the reason why, for a long time, many authors were questioning the correctness of the Rayleigh approach [5]. In 1979 MCPHEDRAN *et al.* [2] pointed out that an infinite, flat layer of a composite subjected to the external temperature gradient is the only correct sample shape for calculation of λ_{ef} by the Rayleigh method.

An interesting approach has been proposed by ZUZOVSKI, BRENNER [6] and SANGANI, ACRIVOS [7]. Their methods avoid all the difficulties of the Rayleigh method mentioned above. They decomposed the temperature field into two components. The first one is a macroscopic shape-dependent component $T^{i,m}$, and the second one is periodic, depending on the geometry and physical properties of the composite $T^{i,p}$,

$$T^i = T^{i,m} + T^{i,p}, \tag{1.8}$$

where $i = c, d$. In view of the periodicity of the temperature field and the square symmetry of the array, the normal derivative of the periodic component of temperature is equal to 0 on the cell boundary,

$$\mathbf{n} \cdot \nabla T^{c,p} = 0, \tag{1.9}$$

where $\mathbf{n}$ is a unit vector normal to the boundary of the cell. Condition (1.9) may be considered as equivalent to the equations of Rayleigh (1.4).

It was shown in [6, 7] that the periodic component may be expressed by an infinite set of derivatives of a certain function T_0 called the Wigner potential [8]. By using these derivatives ZUZOVSKI, BRENNER [6] and SANGANI, ACRIVOS [7] investigated the effective conductivity of regular arrays of spheres. They noticed that successive derivatives of T_0 formed a functional basis convenient for representation of solutions of three-dimensional Laplace equations.

The main aim of this paper is to construct a new functional basis for periodic, two-dimensional potentials generated by the Laplace equation. As an example, we will derive a simple recurrence formula for evaluation of the effective conductivity, in the form of a power series in u, for a square array of circular cylinders.

2. The functional basis

The Rayleigh functional basis consists of multipoles located in the centers of single cells. These basic functions do not fulfill the periodic boundary condition on the boundary of the cell. Our aim is to find a basis, the elements of which fulfill identically the periodicity conditions. Such a basis can be built up with the aid of the Wigner potential. In this section we shall limit our investigation merely to the periodic term $T^{i,p}$ of the temperature field. For the sake of convenience, the upper index p in $T^{i,p}$ will be omitted, i.e. $T^{i,p} \equiv T^i$.

Let us consider an infinite system of point heat sources of intensity q, located in the nodes of a square array of period l, accompanied by neutralizing fuzzy sources of uniform density $\tau = -q/l$ of the opposite sign. In such a grid, the global intensity of sources is equal to 0. The temperature field generated by such a system of sources fulfills the Poisson equation (2.1)

$$\nabla^2 T = -2\pi q \cdot \left(\delta(\mathbf{r}) - \frac{1}{l^2} \right), \tag{2.1}$$

and the boundary condition (1.9), where $\delta(\mathbf{r})$ is the Dirac function. The solution of equations (2.1) and (1.9) was given by CICHOCKI and FELDERHOF [8] in the form:

$$T_0(\mathbf{r}) = q \cdot \left(-\ln r + \frac{1}{2}\pi r^2 + \sum_{m=4}^{\infty} A_m r^m \cos m\theta \right). \tag{2.2}$$

Coefficients A_m were found in the process of summation over an infinite grid of cells, with the exception of the cell located in the center of the coordinate system. Coefficients A_m are related to the Rayleigh sums S_m (1.6) as follows,

$$A_m = \frac{S_m}{m}.$$

The index m in (2.2) is a multiple of 4, because $T_0(\mathbf{r})$ is independent of rotation of the frame of reference by the angle $\pi/2$. The first term in the parentheses of (2.2) represents the influence of a single source located in the center of the cell, the second one is generated by the fuzzy sources, while the third term given by the infinite sum is due to the sources located in the external cells. Function (2.2), called the Wigner potential [8], can be used as a starting point for the construction of the functional basis for periodic two-dimensional potentials.

A multipole of order k includes 2^k point sources, and it is defined by the scalar intensity q_k and k unit vectors $\mathbf{n}_s$, $s = 1, 2, \ldots, k$, representing the directional properties of the multipole (see for example [9]). The multipole potential is proportional to the k-th directional derivative of the point source potential in directions $\mathbf{n}_1, \mathbf{n}_2, \ldots, \mathbf{n}_k$, respectively.

$$T_k(\mathbf{r}) = q_k \cdot \left[\prod_{s=1}^{k} (-1)^k (\mathbf{n}_s \cdot \nabla) \right] T_0(\mathbf{r}), \qquad k = 1, 2, \ldots . \tag{2.3}$$

For a classical multipole, $T_0(\mathbf{r})$ is the potential of a point source in an infinite region: in the 2-dimensional case

$$T_0(\mathbf{r}) = -\ln r. \tag{2.4}$$

Instead of a single multipole, one may consider an infinite system of identical multipoles of order k located in the nodes of a square array. To determine the potential of such a grid, one should apply the operator of the right-hand side of (2.3) to the function $T_0(\mathbf{r})$ defined by (2.2). Positive and negative fuzzy sources balance each other and they have no influence on the global potential.

In the operator $\mathbf{n}_s \cdot \nabla$ of directional derivative, one may distinguish two components of different types of symmetry,

$$\mathbf{n}_s \cdot \nabla = \alpha_s \mathcal{U} + \beta_s \cdot \mathcal{V}, \tag{2.5}$$

where

$$\mathcal{U} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r} \frac{\partial}{\partial \theta},$$
$$\mathcal{V} = \sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r} \frac{\partial}{\partial \theta}.$$

Action of the operator $\mathcal{U}$ on the symmetric or antisymmetric functions produces the results of the same type of symmetry: symmetric or antisymmetric, respectively. On the other hand, operator $\mathcal{V}$ changes the type of symmetry to the opposite one. Let us introduce the notations:

$$T_k^{c,s} = (-1)^k (k-1)! \frac{\cos k\theta}{r^k} + \pi(\delta_{1k} r \cos\theta + \delta_{2k}) + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} r^m A_{k+m} \cos m\theta, \tag{2.6}$$

$$T_k^{c,a} = (-1)^k (k-1)! \frac{\sin k\theta}{r^k} + \pi\delta_{1k} r \sin\theta + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} r^m A_{k+m} \sin m\theta \,. \tag{2.7}$$

The differential operators $\mathcal{U}$ and $\mathcal{V}$ acting on functions $T_k^{c,s}(\mathbf{r})$ and $T_k^{c,a}(\mathbf{r})$ have the following properties:

$$\begin{aligned} \mathcal{U}T_k^{c,s} &= T_{k+1}^{c,s}, \qquad & \mathcal{U}T_k^{c,a} &= T_{k+1}^{c,a}, \\ \mathcal{V}T_k^{c,s} &= T_{k+1}^{c,a}, \qquad & \mathcal{V}T_k^{c,a} &= T_{k+1}^{c,s} 1. \end{aligned} \tag{2.8}$$

Applying the operator $(\mathbf{n}_s \cdot \nabla)$, $s = 1, \ldots, k$, to the function $T_0(\mathbf{r})$ k-times, one obtains a sum of the following terms:

$$\mathcal{U}^j \mathcal{V}^{k-j} T_0(\mathbf{r}), \qquad j = 0, 1, \ldots, k \,;$$

hence

$$T_k(\mathbf{r}) = C_k T_k^{c,s}(\mathbf{r}) + D_k T_k^{c,a}(\mathbf{r}), \tag{2.9}$$

where C_k and D_k are certain known numerical coefficients.

The functions $T_k^{c,s}$ and $T_k^{c,a}$ defined by (2.6) and (2.7) constitute a basis for the solution in the elementary cell outside the cylinder. According to (2.9), the potential of the grid of k-th order multipoles is a linear combination of symmetric and antisymmetric functions of k-th order.

The functions $T_k^{c,s}$ and $T_k^{c,a}$ have singularities on the axis of the cylinder, and they can not be used for representing the solution inside the cylinder. In this region, we assume the basis (2.10), (2.11) without singularity

$$T_k^{d,s} = (-1)^k (k-1)! \frac{r^k}{a^{2k}} \cos k\theta + \pi(\delta_{1k} r \cos\theta + \delta_{2k}) + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} r^m A_{k+m} \cos m\theta \,, \tag{2.10}$$

$$T_k^{d,a} = (-1)^k (k-1)! \frac{r^k}{a^{2k}} \sin k\theta + \pi\delta_{1k} r \sin\theta + \sum_{m=1}^{\infty} \frac{(m+k)!}{m!} r^m A_{k+m} \sin m\theta \,. \tag{2.11}$$

It is easily seen that for $r = a$, the corresponding functions in both the bases are equal,

$$\mathbf{T}_k^{c,s}(a,\theta) = \mathbf{T}_k^{d,s}(a,\theta), \qquad \mathbf{T}_k^{c,a}(a,\theta) = \mathbf{T}_k^{d,a}(a,\theta). \tag{2.12}$$

Representing the solution in the bases (2.6)–(2.7) and (2.10)–(2.11), we fulfill identically the condition (1.9) of periodicity on the cell wall, and continuity of temperature on the cylinder surface. The condition of equality of normal components of a heat flux on the cylinder boundary determine uniquely the coefficients of expansion of λ_{ef} in our basis.

Let us introduce the symbols for the basic functions in both components of the composite:

$$T_k^s = \begin{cases} T_k^{d,s} \\ T_k^{c,s} \end{cases} \qquad T_k^a = \begin{cases} T_k^{d,a} & r \leq a, \\ T_k^{c,a} & r \geq a. \end{cases} \tag{2.13}$$

Derivatives of the functions T_k^s and T_k^a are discontinuous for $r = a$. Both functions (2.13) fulfill the Poisson equations (2.14)–(2.15) given by

$$\nabla^2 T_k^s = -\delta(r-a)\cos k\theta, \tag{2.14}$$

$$\nabla^2 T_k^a = -\delta(r-a)\sin k\theta. \tag{2.15}$$

The relations (2.14)–(2.15) enable another interpretation of the basic functions, as a potential generated by the sources located at the cylinder boundary. The cosine and sine heat sources generate the symmetric functions (2.6) and (2.10), and the antysymmetric functions (2.7) and (2.11), respectively. In this interpretation, the intrinsic ties between the singular functions for the region outside the cylinders and non-singular functions inside the cylinders, are easily seen. For the case of circular cylinders arranged in a square array, the solution of (1.1)–(1.3) is a symmetric function. Hence we shall not consider in the sequel the basic functions T_k^a.

3. Recurrence algorithm

Using the functional basis given by the symmetric functions (2.6) and (2.10), we shall express the temperature field of the matrix ($i = c$) and inclusions ($i = d$), determined by Eqs. (1.1), (1.2) and (1.9), in the form of a power series expansion in u,

$$T^i(r,\theta;\varphi,u) = \tau^{(0)} + \sum_{m=1}^{\infty} \tau^{(i,m)}(r,\theta;\varphi)u^m. \tag{3.1}$$

Here, according to the previous definition (1.8), the function T^i in (3.1) is the sum of both the macroscopic $\tau^{(0)}$ and periodic (the sum for $m \geq 1$) parts of the temperature field. In this respect, the notations of Eqs. (3.1) and (1.8) are different. Following BERGMAN [10], we rewrite Eqs. (1.1) in a form valid for both the matrix and the inclusion in a unit cell,

$$\nabla \cdot (1 + u\theta_d)\nabla T^i = 0, \tag{3.2}$$

where θ_d is the characteristic function of inclusions. By inserting the series (3.1) into Eq. (3.2) and collecting terms with the same power of u, we obtain the general recurence formula for the coefficients $\tau^{(i,m)}$:

$$\begin{aligned} \nabla^2\tau^{(0)} &= 0, \\ \nabla^2\tau^{(i,m)} &= -\nabla\theta_d \cdot \nabla\tau^{(i,m-1)}, \qquad m = 1, 2, \ldots . \end{aligned} \tag{3.3}$$

The composite is subjected to an external temperature gradient equal to unity. Hence the solution of $(3.3)_1$ is given by $\tau^{(0)} = r\cos\theta$.

Now let us turn our attention to the periodic part of the solution determined by Eq. $(3.3)_2$. Taking into account properties of the scalar product and of the characteristic function θ_d, we rearrange its right-hand side and Eq. $(3.3)_2$ takes the form [11]

$$\nabla^2\tau^{(i,m)} = \delta(r-a)\frac{\partial\tau^{d,m-1)}}{\partial r}, \tag{3.4}$$

where the functions $\tau^{(d,m-1)}$ $(m = 1, 2, \ldots)$ are defined inside the cylinder, and a denotes the radius of the cylinder. Note that the functions $\tau^{(i,m)}$ determined by $(3.3)_2$ are periodic and can be represented by the series

$$\tau^{(i,m)} = \sum_{k=1}^{\infty} c_k^{(m)} T_k^i, \qquad \text{for} \quad m = 1, 2, \ldots, \tag{3.5}$$

where T_k^i are the basic functions given by (2.6) and (2.10), while $c_k^{(m)}$ are real coefficients.

Now let us present the basic functions in a renormalized form which will be more convenient for further considerations. Superscript s will be here disregarded since only symmetric basic functions are the subject of our interest,

$$T_j^c = \frac{a^{j+1}}{2j!}\left[(j-1)!\,\frac{\cos j\theta}{r^j} + \sum_{k=1}^{\infty} p_{jk} r^k \cos k\theta\right], \tag{3.6}$$

$$T_j^d = \frac{a^{j+1}}{2j!}\left[(j-1)!\,\frac{r^j}{a^{2j}}\cos j\theta + \sum_{k=1}^{\infty} p_{jk} r^k \cos k\theta\right], \tag{3.7}$$

where

$$p_{jk} = -\frac{(j+k)!}{k!}\left(A_{j+k} + \frac{1}{2}\pi\delta_{j+k,2}\right). \tag{3.8}$$

Inserting (3.5) into (3.4) and making use of (2.14), we obtain the recursion formula for the coefficients $c_k^{(m)}$

$$\sum_{k=1}^{\infty} c_k^{(m+1)} \cos k\theta = -\sum_{j=1}^{\infty} c_j^{(m)} \frac{\partial}{\partial r} T_j^d. \tag{3.9}$$

Next, introducing T_k^d given by (3.7) into (3.9) and collecting the terms with $\cos k\theta$, we finally arrive at:

$$c_k^{(m+1)} = -\sum_{j=1}^{\infty} c_j^{(m)} \left(\frac{1}{2}\delta_{kj} + p_{kj}\frac{ka^{k+j}}{2j!} \right), \qquad k = 1, 2, \ldots, \tag{3.10}$$

where the term p_{jk} is given by (3.8).

The input data for algorithm (3.7) are

$$c_k^{(1)} = \delta_{1k}, \qquad k = 1, 2, \ldots, \tag{3.11}$$

since the gradient of external temperature field is equal to unity. The recurrence formula (3.10) allows us to compute the coefficients $c_k^{(m)}$ ($m = 1, 2, \ldots$) in (3.5), and hence to determine by means of (3.1) the temperature field T^i inside the unit cell.

It is worth to note that the solution of Eqs. (1.1) presented by (3.1) with (3.5)–(3.8) and (3.10) satisfies the boundary conditions (1.2), in spite of the fact that they were not introduced here explicitly. In fact, the boundary condition $(1.2)_1$ is fulfilled owing to the form of the basic functions assumed, what can be seen from Eqs. (2.12). The condition $(1.2)_2$ can be rewritten, with the aid of (1.5), to the following form:

$$\left.\frac{\partial T^c}{\partial r}\right|_{r=a+0} - \left.\frac{\partial T^d}{\partial r}\right|_{r=a-0} = u \left.\frac{\partial T^d}{\partial r}\right|_{r=a-0}. \tag{3.12}$$

Inserting (3.1), (3.5), (3.6) and (3.7) to (3.12) and collecting terms with equal powers of u we get first $c_1^{(1)} = 1$ (see (3.11)), and then the recurrence expression (3.10) for the successive coefficients $c_k^{(m+1)}$. Thus we can see that the procedure presented here satisfies both boundary conditions (1.2).

4. Calculation of effective conductivity

Now we shall use the recurrence algorithm to calculate the effective conductivity of the composite. To this end let us consider the temperature field in the matrix which can be expressed by Eq. (3.1) with the aid of (3.5) and the basic functions (3.6). This expression may be transformed to the Rayleigh form $(1.3)_1$ which allows us to calculate the coefficient b_1 of the term $\cos\theta/r$ of the power series of u. Inserting b_1 into (1.7) we obtain the formula for effective conductivity of the composite

$$\mu(u) = 1 + \sum_{n=1}^{\infty} C_n u^n, \tag{4.1}$$

where

$$C_n = \varphi c_1^{(n)}. \tag{4.2}$$

The coefficients $c_1^{(n)}$ can be obtained from the recurrence formula (3.10) which for $k = 1$ takes the following form

$$c_1^{(m+1)} = -c_1^{(m)}\frac{1}{2}(1-\varphi) + 2\sum_{n=1}^{\infty} c_{4n-1}^{(m)} n A_{4n} (\varphi/\pi)^{4n}, \tag{4.3}$$

while coefficients $c_{4n-1}^{(m)}$ are calculated directly from (3.10).

We start our calculations with (3.11), and then from Eq. (4.3) we obtain the successive coefficients. The first four of them are listed below:

$$c_1^{(1)} = 1, \tag{4.4}$$

$$c_1^{(2)} = -\frac{1}{2}(1-\varphi), \tag{4.5}$$

$$c_1^{(3)} = -c_1^{(2)}\frac{1}{2}(1-\varphi) + 4\sum_{n=1}^{\infty}(4n-1)(nA_{4n})^2(\varphi/\pi)^{4n}, \tag{4.6}$$

$$c_1^{(4)} = -\left[c_1^{(3)}\frac{1}{2}(1-\varphi) + 2(2-\varphi)\sum_{n=1}^{\infty}(4n-1)(nA_{4n})^2(\varphi/\pi)^{4n}\right]. \tag{4.7}$$

The process could be continued, however the expressions for coefficients of higher order are more complex and they will not be presented here. The coefficients of higher order were calculated numerically from the formula (4.3). The first nonvanishing Wigner coefficients A_m which appear in Eqs. (4.3) and (4.6)–(4.7) are given below:

$$A_4 = 0.7878030005, \qquad A_8 = 0.5319716294,$$
$$A_{12} = 0.3282374177, \qquad A_{16} = 0.2509809396.$$

The values of coefficients $C_n(\varphi)$ were obtained from the formula (4.2). Several low order coefficients (up to C_6) are gathered in Table 1.

Now we compare Eq. (4.1) with the Maxwell–Garnett formula (see [11, 12]) which is the first approximation of the effective conductivity coefficient. The Maxwell–Garnett formula may be presented as a function of u and φ in the following form:

$$\mu = 1 + \frac{\varphi u}{1 + u(1-\varphi)/2}. \tag{4.8}$$

Table 1. Coefficients of the power series expansion of effective conductivity μ for a square array of cylinders.

φ	C_1	C_2	C_3	C_4	C_5	C_6
0.10	0.10	−0.04500	0.020250	−0.009113	0.004101	−0.001846
0.20	0.20	−0.08000	0.032024	−0.012830	0.005148	−0.002068
0.30	0.30	−0.10500	0.036936	−0.013086	0.004682	−0.001698
0.40	0.40	−0.12000	0.036784	−0.011662	0.003884	−0.001381
0.50	0.50	−0.12500	0.033646	−0.010208	0.003615	−0.001488
0.60	0.60	−0.12000	0.029979	−0.010181	0.004465	−0.002255
0.70	0.70	−0.10500	0.028735	−0.012751	0.006975	−0.004169
0.75	0.75	−0.09375	0.030114	−0.015261	0.009200	−0.006077

If we expand (3.20) into a power series of u, we obtain

$$\mu = 1 + \varphi\left[u - \frac{1}{2}(1-\varphi)u^2 + \frac{1}{4}(1-\varphi)^2u^3 - \frac{1}{8}(1-\varphi)^3u^4 + \ldots\right]. \tag{4.9}$$

Although this expression (4.9) is only a rough approximation of μ, certain resemblance to the formula (4.1) and (4.2)–(4.7) can easily be seen. In fact, the coefficients at the first and the second power of u which appear in (4.9), and those calculated from (4.4) and (4.5), are identical. The other coefficients of (4.9) are identical merely with the leading terms of the expressions (4.6) and (4.7).

5. Continued fraction expansion

The power series expression (4.1) is not an effective form for representing μ because of the small convergence radius and very slow rate of convergence. It is much better to express $\mu(\varphi, u)$ in the form of a continued fraction (see [11, 12]). Comparison of the two forms (4.8) and (4.9) illustrates how convenient and effective may be the rational representation, as compared with infinite series.

If we substitute $s = 1/u$ into Eq. (4.1), we can present the series in the form of a J-fraction [13]

$$\mu(\varphi, s) = 1 + \frac{k_1}{l_1 + s -}\,\frac{k_2}{l_2 + s -}\,\frac{k_3}{l_3 + s -}\,\frac{k_4}{l_4 + s -}\,\ldots, \tag{5.1}$$

where coefficients $k_n(\varphi)$ and $l_n(\varphi)$ can be determined using the coefficients C_n (Table 1), on the basis of another recurrence algorithm given in the Appendix.

The coefficients of the first level of the J-fraction calculated in the Appendix (A.4) are

$$k_1 = \varphi, \qquad l_1 = (1-\varphi)/2. \tag{5.2}$$

Inserting (5.2) into (5.1) and assuming the other coefficients to be equal to zero, we get

$$\mu = 1 + \frac{\varphi}{(1-\varphi)/2 + 1/u} = 1 + \frac{\varphi u}{u(1-\varphi)/2 + 1}\,. \tag{5.3}$$

We can see that Eq.(5.3) is identical with the Maxwell-Garnett formula (4.8), the accuracy of which is limited to small values of u and φ. However, it is an advantageous feature of the continuous fraction expansion that successive approximants of the fraction rapidly increase its accuracy. The results presented in [11] indicate that for $u \to \infty$ and $\varphi = 0.7$, which is a rather high value, only three or four levels of the fraction are sufficient to preserve a good accuracy. Nevertheless in the asymptotic case, if $\varphi \to \varphi_{\max} = \pi/4$, the method presented here fails and an analysis of a different kind is needed [14].

In the present paper the algorithm has been applied to a composite which consists of a square array of cylinders embedded in a matrix. The algorithm was also applied to the composites of hexagonal geometry [15].

6. Conclusion

A new functional basis derived in this paper allowed us to obtain a simple recurrence algorithm for calculating the effective transport coefficient of regular two-dimensional composites (3.10), (3.11). The algorithm is simply recursive and does not involve the solution of a large number of coupled equations. The results are used as input data to express the effective transport coefficient in the form of a rapidly convergent continuous fraction expansion.

Appendix

The algorithm presented below enables a recurrence calculation of the J-fraction coefficients k_n and l_n, on the basis of the given coefficients C_n of the power series (4.1). The coefficients are calculated from the following formulae [13]:

$$k_{n+1} = \frac{\sigma_n}{\sigma_{n-1}}\,, \qquad l_{n+1} = \tau_{n-1} - \tau_n\,, \tag{A.1}$$

where

$$\sigma_n = C_{2n+1} + \sum_{j=1}^{n} b_{nj} C_{2n+1-j}\,, \tag{A.2}$$

$$\tau_n = \frac{1}{\sigma_n}\left[C_{2n+2} + \sum_{j=1}^{n} b_{nj} C_{2n+2-j}\right]. \tag{A.3}$$

We start with $n = 0$. The required initial values of parameters are

$$\sigma_{-1} = 1, \qquad \tau_{-1} = 0.$$

Hence we have from (A.1)–(A.3)

$$k_1 = C_1 = \varphi, \qquad l_1 = -\frac{C_2}{C_1} = \frac{1}{2}(1-\varphi). \tag{A.4}$$

The successive values of k_n, l_n are then calculated from (A.1). Several auxiliary parameters b_{nj} in (A.2) and (A.3) have the following values:

$$b_{n-1,-1} = 0, \qquad b_{n,n+1} = 0, \qquad b_{n+1,0} = 1, \qquad b_{0,0} = 1,$$

the other ones must be determined from the relation

$$b_{n,j} = b_{n-1,j} + l_n b_{n-1,j-1} - k_n b_{n-2,j-2}\,. \tag{A.5}$$

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References

1. J.W. RAYLEIGH, *On the influence of obstacles arranged in rectangular order on the properties of the medium*, Phil. Mag., Ser. 5, **34**, 481–502, 1892.
2. W.T. PERRINS, D.R. MC KENZIE and R.C. MC PHEDRAN, *Transport properties of regular arrays of cylinders*, Proc. R. Soc. London, A **369**, 207–225, 1979.
3. R.C. MC PHEDRAN and D.R. MC KENZIE, *Electrostatic and optical resonances of arrays of cylinders*, Appl. Phys., **23**, 223–235, 1980.
4. R.C. MC PHEDRAN and G.W. MILTON, *Bounds and exact theories for the transport properties of inhomogeneous media*, Appl. Phys., A **26**, 207–220, 1981.
5. D.J. JEFFREY, *Conduction through a random suspension of spheres*, Proc. R. Soc. London, A **335**, 355–367, 1973.
6. M. ZUZOVSKY and H. BRENNER, *Effective conductivities of composite materials composed of cubic arrangements of spherical particles embedded in an isotropic matrix*, ZAMP, **28**, 6, 979–992, 1977.
7. A.S. SANGANI and A. ACRIVOS, *The effective conductivity of a periodic array of spheres*, Proc. R. Soc. London, A **386**, 263–275, 1983.
8. B. CICHOCKI and B.U. FELDERHOF, *Electrostatic spectrum and dielectric constant of nonpolar hard sphere fluids*, J. Chem. Phys., **90**, 9, 1989.
9. C.J.F. BÖTTCHER, *Theory of electrical polarization*, 2-nd Ed., Amsterdam 1973.
10. D.J. BERGMAN, *The dielectric constant of a composite material – a problem in classical physics*, Physics Reports, C **43**, 378–407, 1978.

11. S. MAY, S. TOKARZEWSKI, A. ZACHARA and B. CICHOCKI, *Effective conductivity of a two-component composite with a regular two-dimensional structure* [in Polish], IFTR Reports, **24**, 1992.

12. S. MAY, S. TOKARZEWSKI, A. ZACHARA and B. CICHOCKI, *Continued fraction representation for the effective thermal conductivity coefficient of a regular two-component composite*, Int. J. Heat and Mass Transf., **37**, 2165–2173, 1994.

13. W.D. JONES and W.J. THORN, *Continued fractions. Analytic theory and its applications*, [in:] Encyclopedia of Mathematics and its Applications, vol. **11**, Addison-Wesley Publ. Co., 1980.

14. S. TOKARZEWSKI, J. BŁAWZDZIEWICZ and I.V. ANDRIANOV, *Effective conductivity of densely packed highly conducting cylinders*, Appl. Phys. A, 601–604, 1994.

15. S. TOKARZEWSKI and J.J. TELEGA, *S-continued fraction representation for effective transport coefficients of two-phase media*, IFTR Reports, **16**, 1995.

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