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Two-point quasifractional approximants for effective conductivity of a simple cubic lattice of spheres

I. ANDRIANOV and V. DANISHEVSKYI
Civil Engineering Institute, Dnepropetrovsk, Ukraine

and

S. TOKARZEWSKI
Center of Mechanics, Institute of Fundamental Technological Research, Warsaw, Poland

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Abstract—We study the effective heat conductivity k of a periodic cubic array (with side length l) of perfectly conducting spheres of the volume φ, embedded in a matrix material with conductivity 1. We construct a sequence of quasifractional approximants for the effective conductivity. As the bases for the construction we use the perturbation approach for $\varphi \to 0$ and asymptotic formula for $\varphi \to \pi/6$ (limiting value of sphere) and as a tool—quasifractional approximants. Copyright © 1996 Elsevier Science Ltd.

1. INTRODUCTION

One of the main tasks of the theory of dispersed media is a theoretical prediction of the effective transport properties. The subject we discuss in this paper has a long history dating back to J. C. Maxwell (1873). The problem may be formulated in a number of mathematically equivalent ways, but here we shall discuss it in the language of heat conductivity: we wish to determine the effective conductivity of an infinite simple cubic lattice of identical macroscopic, perfect conducting spheres, immersed in a matrix. In ref. [1] is displayed a table showing light distinct physical problems which may be solved by analogous mathematical methods. One of these is the above mentioned conductivity problem, while others involve calculating the dielectric constant, the magnetic permeability, electric conductivity, elastic constants, etc.

The calculation of k for a general type of composite was originally discussed by Maxwell (1873) and subsequently has been considered by many others. The solution for the case of small spheres was first examined by Rayleigh (1892), who described the polarization of each sphere in an external field by an infinite set of multipole moments. This method has recently been extended, with the aid of modern digital computers, so that a large number of multipoles can now be calculated [2, 3]. A historical review of the subject, including an exhaustive list of references, was recently compiled in ref. [4].

The power-series expansion has been used to construct Pade-approximants and continued fraction representation of the effective conductivity in refs. [5, 6]. Pade approximants are successfully used in the theory of composite materials as calculations of the effective constants and for estimation of the upper and lower bounds for it [5]. Neither of the above mentioned methods yields accurate results for a system of perfectly conductive, nearly touching spheres. In order to describe such a system in ref. [7] an asymptotic formula is derived. However, the validity range of this formula is not known. However, there still remains a certain parameter range which is covered neither by the asymptotic formula nor by the solutions based assumption of small φ.

Practically any physical or mechanical problem, whose parameters include the variable parameter ε, can be approximately solved as it approaches zero, or infinity. How can this 'limiting' information be used in the study of a system at the intermittent values of ε? This problem is one of the most complicated in asymptotic analysis. In many instances the answer to it is alleviated by two-point Pade approximants [8, 9].

As shown in ref. [10], two-point Pade approximants may be effectively used for the study of the effective heat conductivity λ of a periodic square array of nearly touching cylinders of the conductivity λ_1, embedded in a matrix material of the conductivity λ_0. It was constructed as a sequence of two-point Pade approximants for the effective conductivity of the system. As an input we use the coefficients of the expansion of λ in powers of the parameter $z = (\lambda_1 - \lambda_0)/\lambda_0$ and the value of λ for $z \to \infty$. The two-point Pade approximants form a sequence of rapidly converging upper and lower bounds on the effective conductivity. The

NOMENCLATURE

k	effective thermal conductivity of a composite material
z	auxiliary dimensionless parameter characterizing conductivities of components of a composite material, $(\lambda_1-\lambda_0)/\lambda_0$.
Greek symbols	
λ	effective heat conductivity of the composite material with cylindrical inclusions
λ_1	heat conductivity of cylindrical inclusions
λ_1	heat conductivity of cylindrical inclusions
λ_0	heat conductivity of a matrix material
ψ	volume fraction of dispersed spheres
χ	auxiliary parameter characterizing volume fraction of dispersed spheres, $1-(6\psi/\pi)^{1/3}$.

convergence is much better than in the case of Pade approximants discussed in the literature.

Unfortunately, the asymptotic formula obtained in ref. [7] contains the logarithmic function; that's why two-point Pade approximants in its 'pure form' can't be used in the problem under consideration.

This problem is the most essential for two-point Pade approximants, because as a rule, one of the limits ($\varepsilon\to 0$ or $\varepsilon\to\infty$) for real mechanical problems gives expansions with logarithmic terms or other complicated functions. It is worth noting that in some cases these obstacles may be overcome by using an approximate method of two-point Pade approximant construction by taking as limit points some small and large (but finite) values [11], not $\varepsilon = 0$ and $\varepsilon = \infty$. On the other hand in the last few years, so called quasifractional approximants, which give possibility to the overcoming of the above mentioned obstacles, are widely used in physics [12].

The main purpose of our paper is to fill in this gap. To this end we develop a new approach based on an application of quasifractional approximants. We construct it by using the coefficients of the perturbation expansions of k at $\varphi = 0$ and asymptotic formula for $\varphi\to\pi/6$. This paper is organized as follows: in Section 2 we define the perturbative and asymptotic solutions. A description of our procedure is given in Section 3. In Section 4 we present numerical results and in Section 5 we discuss the advantages and limitations of our method in the light of the results from the previous sections.

2. PERTURBATIVE AND ASYMPTOTIC SOLUTIONS

Maxwell was the first to calculate the effective thermal conductivity k of a composite material volume fraction of dispersed spheres $\varphi \ll 1$. For a perfectly conducting sphere

$$k = 1-3\varphi(\varphi-1)^{-1}. \tag{1}$$

Rayleigh extended this analysis to the case where the spheres are arrayed in a simple cubic lattice, obtaining for perfect conducting spheres

$$k = 1-3\varphi[\varphi-1+\alpha\varphi^{10/3}+0(\varphi^{14/3})]^{-1},\quad \alpha = \text{const.} \tag{2}$$

Rayleigh gave the value $\alpha = 1.65$. This was later corrected by Runge to 0.523.

Sangani and Acrivos [3] obtained the following expression for perfectly conducting spheres

$$k = 1-3\varphi[\varphi-1+1.3047\varphi^{10/3}(1+0.2305\varphi^{11/3})/(1-0.4054\varphi^{7/3})+0.07231\varphi^{14/3}+0.1526\varphi^{6}+0.0105\varphi^{22/3}+0(\varphi^{26/3})]^{-1}. \tag{3}$$

Expressions (1)–(3) give us perturbation solutions for $\varphi \ll 1$.

In their turn Batchelor and O'Brien [7] showed that for perfectly conducting spheres and φ tending to the limit value $\pi/6$, the effective conductivity k has the following asymptotic form ($\chi = 1-(6\varphi/\pi)^{1/3}\to 0$) (see also ref. [3]):

$$k_\alpha = 0.5\pi\ln\chi-0.7. \tag{4}$$

Some numerical results are displayed in Fig. 1. As one can easily see, taking into account the term of higher order in the perturbation series does not lead to a satisfactory agreement between the exact and perturbative solutions. In this turn the asymptotic solution can't be used for small φ. This is the heuristic reason for the attempt of matching the perturbative and asymptotic solutions.

3. QUASIFRACTIONAL APPROXIMANTS

Now we go to the problem of evaluating the effective conductivity in terms of quasifractional approximants [12]. So, we will consider a function determined by a power series expansion at zero and having an asymptotic expansion at infinity. We are now in a

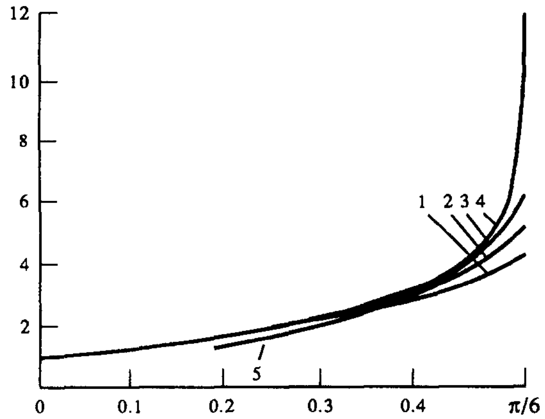

Fig. 1. Effective conductivity λ of a simple cubic array of perfectly conducting spheres as a function of volume fraction φ. The order of the theory is indicated. Numbers 1–5 correspond to the theories of Maxwell [formula (1)], Rayleigh [formula (2)], Sangani and Acrivos [3] [formula (3)], exact value (McKenzie and McPhedran [13]) and asymptotic formula of Batchelor and O'Brien [7].

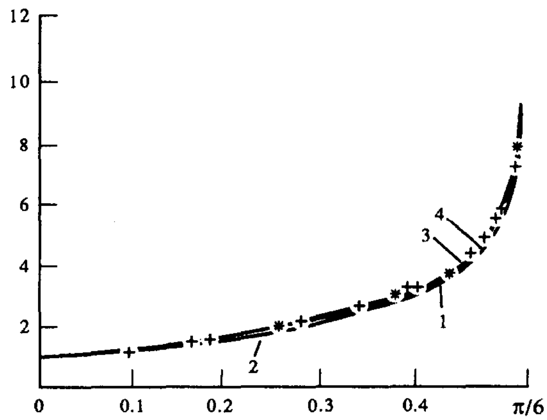

Fig. 2. The experimental measurements of Kharadly and Jackson [14] (+) and of Meredith and Tobias [15] (*) are compared with the quasifractional approximants equations (5), (6), Keller's empirical formula [16] equation (7) and exact theoretical curve [13] (curve 1, 2, 3 and 4 respectively).

position to introduce the quasifractional approximants of the effective conductivity. By definition, the quasifractional approximant, in our case, is a ratio R, the coefficients of which are chosen in such a way that: (a) the expansion of R in powers of φ coincides with the corresponding perturbation expansion of k, equation (3), to the some order and (b) the asymptotic behavior of R coincides with the asymptotic expression (4).

4. ANALYTICAL AND NUMERICAL RESULTS

We now present results for the effective conductivity coefficient, which were obtained by using quasifractional approximants, introduced in the preceding section.

Quasifractional approximants for our case may be written as follows:

$$k = (1+2\varphi+\varphi^{8/3}k_{\alpha}/\chi)/(1-\varphi+\varphi^{8/3}/\chi) \qquad (5)$$

On the other hand, we may construct the approximation as a logarithm of rational function in such a way that its perturbative expansions ($\varphi \to 0$) and asymptotics for $\chi \to 0$ coincide with formulas (2) and (4), respectively.

$$k = -0.5\pi \ln [(0.33883-1.00121\varphi + 0.765364\varphi^2+\varphi^{8/3}/(1-1.2407\varphi^{1/3}))/ (1-1.045035\varphi+0.349038\varphi^2+\varphi^{8/3}/ (1-1.2407\varphi^{1/3}))^2]-0.7 \qquad (6)$$

Some numerical results are displayed in Fig. 2. For comparison we also show the empirical formula by Keller [16]

$$k = -0.5\pi \ln (\pi/6-\varphi) \qquad (7)$$

As mentioned in ref. [7], this formula gives a good agreement with the exact solution, but can't give correct asymptotic behaviour for $\varphi \to 0$.

It is clear that formula (5) better describes the solution for $\varphi \to 0$ and formula (6) is better for $\chi \to 0$, but the discrepancy between them is not large, and this fact justifies the above mentioned procedure.

5. CONCLUDING REMARKS, PERSPECTIVES AND PROBLEMS

The main advantages of the two-point Pade approximants and quasifractional approximants are the simplicity of the algorithms and the possibility of using only a few terms of the expansions. Besides, it is possible to take into account the known singularities of the defined functions.

On the other hand, one of the important problems of using two-point Pade approximants and quasifractional approximants is the control of the accuracy of the realized matching. Sometimes we can use numerical or approximate analytical methods. Along with the comparison of known numerical or analytical solutions, or numerical and experimental results, it is also possible to verify the modified expansions by their mutual correspondence.

Evidently two-point Pade approximants and quasifractional approximants are not a panacea, and in some cases they fail. In these cases it is possible to apply other methods of interpolation.

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