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Simulations of representative volume elements for random 2D composites with circular non–overlapping inclusions

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Abstract: Consider two-dimensional two-component periodic composite made from a collection of non-overlapping, identical, circular disks, embedded in a matrix. In accordance with a theory of the representative cells (representative volume elements), the effective conductivity of disks is expressed in terms of the generalized Eisenstein–Rayleigh sums (ER sums). Straightforward computation of the ER sums is possible only for the sums of lower orders. In the present paper, a fast algorithm to compute higher order sums worked out by use of random walks and Monte Carlo simulations. The algorithm is recurrent, i.e., an ER sum of the fixed order is expressed in terms of the ER sums of lower orders by simple formulae. Relations between the Eisenstein and Weierstrass functions and algebraic dependences between their derivatives are also used to improve the algorithm. The obtained numerical results are applied to investigation of the structure of composites.

Keywords: representative volume element, composite material, Eisenstein–Rayleigh sums

1. Introduction

One of the most important notion of the theory of composites is the representative volume element (RVE). A physical–engineering definition of the RVE can be given as follows [5]. RVE is a part of material which is small enough from a macroscopical point of view and can be thus treated as a typical element of the heterogeneous medium. On the other hand, it is sufficiently large in the microscopical scale, and it represents typical microstructure of the material under consideration. According to this definition one should follow the following scheme to determine the RVE. First, geometric measurements or computations should be made for a class of composites to describe its geometrical characteristics. Second, a number of the real or computational experiments

should be performed to determine the macroscopic tensor property of composites. Third, to compare the results and to make conclusions concerning RVE. The above physical–engineering scheme looks natural but it is not so simple in applications.

A rigorous mathematical theory of the representative cell was proposed in [8]. This mathematical theory is developed now for two–dimensional composites with circular inclusions and outlined for general three–dimensional elastic composites. It is based on the advanced topics of complex analysis but it is simple in applications because one can avoid solution to the boundary value problems at the second step of the physical–engineering approach and simplify the third step by reduction the whole problem to investigation of the generalized Eisenstein–Rayleigh sums introduced below in Sec. 1

It was established in [8] that the effective conductivity tensor Λ_e of the considered composites has the form of double series on the concentration of inclusions and on "basic elements" which depend only on locations of the inclusions. These basic elements are written in terms of the Eisenstein series. Coefficients in the double series depend on conductivity of constitutes. Two composites are equivalent if expansions of their Λ_e have the same basic elements. Therefore, the set of the composites with circular identical inclusions is divided onto classes of equivalence determined only by geometrical structure of the composite. Each composite is represented by a periodicity cell. In each class of equivalence a composite having the minimal size cell is chosen. This cell is called the representative cell of the considered class of equivalent composites.

This approach was used in [4] to investigate the effective transport properties of randomly 2D composites with non–overlapping disks uniformly distributed in a cell. In this case, the effective conductivity tensor is represented in the form $\Lambda_e = \widehat{\lambda} I$, where I denotes the identity matrix and the scalar $\widehat{\lambda}$ the effective conductivity. Let ν stands for the concentration of disks in the cell. The effective conductivity can be considered as a function $\widehat{\lambda}(\nu)$. It was obtained with the accuracy $O(\nu^5)$. For instance, the following formula for perfectly conducting disks was deduced by use of the Padé approximation

$$\widehat{\lambda}(\nu) \approx \frac{3.223}{\nu - 1.247} - \frac{3.237}{\nu - 0.9069} + \frac{0.014\nu + 0.001}{\nu^2 + 0.261\nu + 0.076} \tag{1}$$

This formula is based on computations of the lower multi–index order generalized Eisenstein–Rayleigh sums (ER sums).

In the present paper, we present a fast algorithm to compute the ER sums of higher orders. A method of random walks to simulate random locations of inclusions with high concentrations is applied. The initial locations of disks are fixed in various periodical nodes: square, hexagonal and rectangular. The results show that lower order ER sums which essentially impact on the effective conductivity tensor do not depend on the choice of the original location. But some higher order ER sums "remember" the initial location. This yields the second application of the mathematical theory [8]. It is possible not only to reconstruct the representative cell by pure geometrical data, but also to describe an

engineering method of its creation. For instance, the original regular location of inclusions can be restored for dispersed composites produced by stirring. This observation can be explained by the different scales of convergence of the ER sums during stirring to the limit values when time of random walks tends to infinity. This method also gives a quantitative stirring measure of inclusions in bulk material.

2. Random walk model

Let ω_1 and ω_2 be the fundamental pair of periods on the complex plane $\mathbb{C}$ such that $Im\ \frac{\omega_2}{\omega_1} > 0$. The fundamental parallelogram Q is defined by its vertices $\pm\frac{\omega_1}{2}$ and $\pm\frac{\omega_2}{2}$. Without loss of generality the area of Q can be normalized to one. The points $m_1\omega_1 + m_2\omega_2$ $(m_1, m_2 \in \mathbb{Z})$ generates a doubly periodic lattice $\mathcal{Q}$. Here, $\mathbb{Z}$ stands for the set of integer numbers. Let i denote the imaginary unit. In the case $\omega_1 = \sqrt[4]{\frac{4}{3}}$ and $\omega_2 = \sqrt[4]{\frac{4}{3}}\ e^{\frac{\pi i}{3}}$, the cell Q becomes a rhombus with an angle 60^0 and the array $\mathcal{Q}$ is called the hexagonal lattice (the equilateral triangular lattice).

Consider N non–overlapping circular disks D_k of radius r with the centres $a_k \in Q$ (see Fig. 1). Let D_0 be the complement of all closure disks $|z - a_k| \leq r$ to the domain Q. We study conductivity of the doubly periodic composite when the host $\cup_{m_1,m_2}(D_0 + m_1\omega_1 + m_2\omega_2)$ and the inclusions $D_k + m_1\omega_1 + m_2\omega_2$ are occupied by conducting materials. It is assumed that inclusions are occupied by a perfect conductor that correspond to real fibre composites.

The concentration of the inclusions has the form $\nu = N\pi r^2$. The centres a_k are considered as random variables distributed in such a way that the disks $D_k = \{z \in \mathbb{C} : |z - a_k| < r\}$ generate a set of uniformly distributed non–overlapping disks. Theoretically this distribution denoted below as $\mathcal{U}$ can be introduced as the distribution of the variable $\mathbf{a} = (a_1, a_2, \cdots, a_N) \in Q^N$ with the restrictions $|a_m - a_k| > 2r$ for $m \neq k$ $(m, k = 1, 2, \ldots, N)$. According to [9], $0 \leq \nu \leq \frac{\pi}{\sqrt{12}}$ where $\frac{\pi}{\sqrt{12}}$ is the maximal concentration attained for the hexagonal array. It is worth noting that the disks D_k belong to Q in the torus topology when the opposite sides of Q are identified.

A constructive description of the distribution $\mathcal{U}$ for high concentrations is based on random walks. Put the centres a_k onto the nodes of a regular array. Take a positive number d less than $\min_{k\neq m}|a_k - a_m| - 2r$. Let each a_k moves in a randomly chosen direction $\phi_k \in [0, 2\pi)$ with the step d in the torus topology of Q. Then, each center obtain new complex coordinate $a'_k = a_k + de^{i\phi_k}$. This move is repeated with renewed coordinates for each $k = 1, 2, \ldots, N$ if $|a'_k - a_m| \geq 2r$ (for all $m = k+1, k+2, \ldots, N$). If $|a'_k - a_m| < 2r$ for some m, the point a_k does not move at this step, and we say that it is blocked. After sufficiently large number of the walks the obtained location of the centres can be considered as a statistical realization of the distribution $\mathcal{U}$. This method

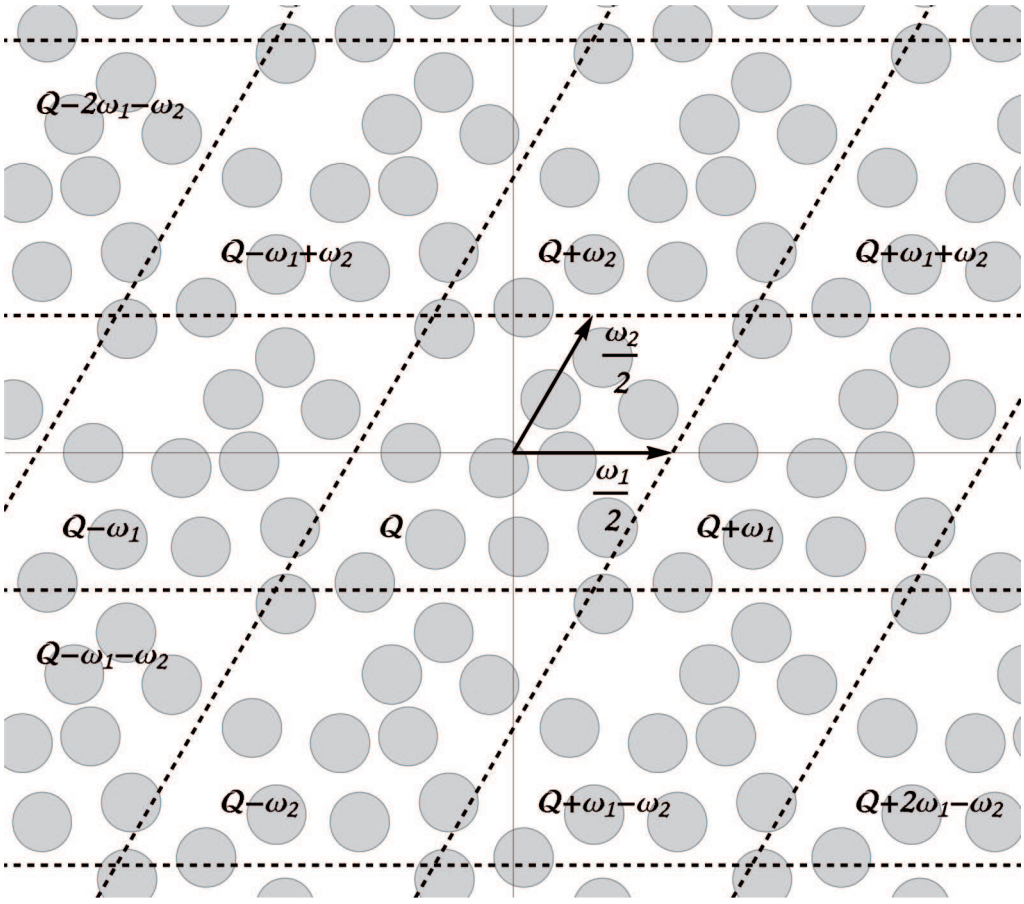

Fig. 1. Doubly periodic composite with inclusions $D_k + m_1\omega_1 + m_2\omega_2$ where $m_1, m_2 \in \mathbb{Z}$

can be applied for arbitrary concentrations satisfying $0 \leq \nu \leq \frac{\pi}{\sqrt{12}}$.

In all computer simulations, we take

$$d = \frac{1}{5}\left(\frac{\omega_1}{\sqrt{N}} - 2r\right) \tag{2}$$

This is the maximal reasonable value of d for which computations are not too frequently blocked for ν not closed to $\frac{\pi}{\sqrt{12}}$. Less value of d decrease the velocity of walking, hence, increase the computation time. However for higher concentrations about $\frac{\pi}{\sqrt{12}}$, computations are frequently blocked for any choice of d. To overcome this difficulty we introduce the maximal number of random choices of the angle ϕ_k, denoted below by P.

After a number of experiments we have taken the following parameters to optimize computations in precision and in time. For each fixed N and ν we calculate r, d and

introduce $P = 1, 2$ or 3. Every center a_k has P attempts to move to a'_k with a randomly chosen direction in each attempt. If it is done for all $k = 1, 2, \ldots, N$, we say that a cycle is performed. The number of cycles is always taken equal to 80. As a result, we have one ultimate location $\mathbf{a} = (a_1, a_2, \ldots, a_N)$. The total number of locations is denoted by M.

3. Computation of Eisenstein-Rayleigh sums

3.1. General theory

Following [7,8] we present constructive formulae for the Eisenstein-Rayleigh sums S_m and the Eisenstein functions $E_m(z)$ corresponding to the lattice $\mathcal{Q}$.

The Eisenstein-Rayleigh lattice sums S_m can be easily calculated through the rapidly convergent series

$$S_2 = \left(\frac{\pi}{\omega_1}\right)^2 \left(\frac{1}{3} - 8\sum_{m=1}^{\infty} \frac{mq^{2m}}{1-q^{2m}}\right), \quad \text{where } q = \exp\left(\pi i\, \frac{\omega_2}{\omega_1}\right), \tag{3}$$

$$S_4 = 60\left(\frac{\pi}{\omega_1}\right)^4 \left(\frac{4}{3} + 320\sum_{m=1}^{\infty} \frac{m^3 q^{2m}}{1-q^{2m}}\right), \tag{4}$$

$$S_6 = 1400\left(\frac{\pi}{\omega_1}\right)^6 \left(\frac{8}{27} - \frac{448}{3}\sum_{m=1}^{\infty} \frac{m^5 q^{2m}}{1-q^{2m}}\right). \tag{5}$$

S_{2n} ($n \geq 4$) can be calculated by the recurrent formula

$$S_{2n} = \frac{3}{(2n+1)(2n-1)(n-3)} \sum_{m=2}^{n-2} (2m-1)(2n-2m-1) S_{2m} S_{2(n-m)}. \tag{6}$$

The rest sums vanish.

The Eisenstein functions [10] are related to the Weierstrass function $\wp(z)$ [1] by the identities

$$E_2(z) = \wp(z) + S_2, \quad E_m(z) = \frac{(-1)^m}{(m-1)!} \frac{d^{m-2}\wp(z)}{dz^{m-2}}, \quad m = 3, 4, \ldots. \tag{7}$$

Every function (9) is doubly periodic and has a pole of order m at $z = 0$. The Eisenstein functions of the even order $E_{2m}(z)$ can be presented in the form of the series [10]

$$E_{2m}(z) = \frac{1}{z^{2m}} + \sum_{k=1}^{\infty} \sigma_k^{(m)} z^{2(k-1)}, \tag{8}$$

where

$$\sigma_k^{(m)} = \frac{(2m+2k-3)!}{(2m-1)!(2k-2)!} S_{2(m+k-1)}. \tag{9}$$

We follow [8] to introduce the generalized Eisenstein-Rayleigh sums. Let a_k ($k = 1, 2, \ldots, N$) be a set of points. Let q be a positive integer; k_t runs over 1 to N; $m_j = 2, 3, \ldots$. Let $\mathbf{C}$ be the operator of complex conjugation. Introduce the following sum of multi-index $(m_1, \ldots, m_q)$

$$\begin{aligned} e_{m_1 \ldots m_q} := N^{-[1+\frac{1}{2}(m_1+\cdots+m_q)]} \sum_{k_0 k_1 \ldots k_q} E_{m_1}(a_{k_0} - a_{k_1}) \\ \times \overline{E_{m_2}(a_{k_1} - a_{k_2})} \ldots \mathbf{C}^q E_{m_q}(a_{k_{q-1}} - a_{k_q}). \end{aligned} \tag{10}$$

Here, it is assumed for convenience that

$$E_m(0) := S_m. \tag{11}$$

According to (10)–(11), e_m becomes the classical Eisenstein-Rayleigh sum S_m in the case $N = 1$. The following useful formula was proved in [4]

$$e_{m_1 \ldots m_q} = (-1)^{\sum_{j=1}^q m_j} \mathbf{C}^q e_{m_q \ldots m_1} \tag{12}$$

The sums (10) constitute the basic elements dependent only on locations of inclusion. The effective conductivity tensor is presented as a linear combinations of (10) with coefficients dependent on the physical properties of constitutes and the concentration [8,3.6]. Let an accuracy in the concentration $O(\nu^p)$ is fixed. Then a finite set $\mathcal{M}_p$ of the basic elements (10) is needed to identify a representative cell [8].

3.2. Algorithm

Straightforward computation of the sums (10) is based on the standard summation formula

$$\sum_{k_0=1}^N \sum_{k_1=1}^N F_1(a_{k_0} - a_{k_1}) \sum_{k_2=1}^N F_2(a_{k_1} - a_{k_2}) \sum_{k_3=1}^N F_3(a_{k_2} - a_{k_3}) \cdots \sum_{k_q=1}^N F_q(a_{k_{q-1}} - a_{k_q}). \tag{13}$$

They are expensive for large N and q.

We describe now a fast recurrent algorithm to compute the sums (10) of order $(m_1 \ldots m_q)$ by use of the sums of lower orders. Introduce the matrix

$$C_s = \begin{pmatrix} F_s(a_1 - a_1) & F_s(a_1 - a_2) & \cdots & F_s(a_1 - a_N) \\ F_s(a_2 - a_1) & F_s(a_2 - a_2) & \cdots & F_s(a_2 - a_N) \\ \vdots & \vdots & \ddots & \vdots \\ F_s(a_N - a_1) & F_s(a_N - a_2) & \cdots & F_s(a_N - a_N) \end{pmatrix}. \tag{14}$$

Introduce the product of matrices

$$C_1 C_2 \dots C_q \tag{15}$$

One can see that the sum of the components of the matrix (15) is equal to the sum (13).

We propose the following algorithm based on formulae (14)-(15). Let $O(\nu^p)$ be a fixed accuracy in the theory of representative cells.

- The set $\mathcal{M}_p$ of multi-indexes $(m_1, \dots, m_q)$ is generated to reach the accuracy $O(\nu^p)$ in accordance with [8].
- All the matrices (14) with $s \in \mathcal{M}_p$ are computed and put into storage.
- The sums (13) are computed by summation of the elements of the product matrix (15).

Table 1 contains the number of elements of $\mathcal{M}_p$ in the first line. For instance, the

accuracy	$O(\nu^5)$	$O(\nu^6)$	$O(\nu^7)$	$O(\nu^8)$	$O(\nu^9)$	$O(\nu^{10})$
number of terms	8	16	32	64	128	256
reduced number	7	13	23	43	79	151
accuracy	$O(\nu^{11})$	$O(\nu^{12})$	$O(\nu^{13})$	$O(\nu^{14})$	$O(\nu^{15})$	$O(\nu^{16})$
number of terms	512	1024	2048	4096	8192	16384
reduced number	287	559	1087	2143	4223	8383

Table 1. Number of elements of $\mathcal{M}_p$ and reduced number of elements after application of (12) for given accuracy.

accuracy $O(\nu^5)$ yields 8 terms e_2, e_{22}, e_{33}, e_{222}, e_{44}, e_{332}, e_{233}, e_{2222}. But application of (12) reduces the number of terms to 7. Here, the terms e_{332} and e_{233} are related by (12). One can see that the reduced number of terms is less than the initial number approximately in 2 times for large p.

The functions $F_s(z)$ in (14) are even or odd. This also reduces the computation of C_s by restriction to a triangular matrix. Moreover, the Eisenstein functions (9)-(10) are expressed by the Weierstrass function $\wp(z)$ and its derivatives. It follows from the theory of elliptic functions [10] that all the derivatives of $\wp(z)$ are algebraically expressed through $\wp(z)$ and $\wp'(z)$ that also accelerates the computations.

Comparison of the CPU time for the standard method and our modification is presented in Fig. 3. Symbolic computations were performed in *Mathematica*® with the use of **Sum** operator.

3.3. Initial locations for random walks

The hexagonal, square and rectangular lattices are considered (see Fig. 4) with the concentration $\nu = 0.6$ as initial locations of the points a_k and further random walks described in Sec. 2.

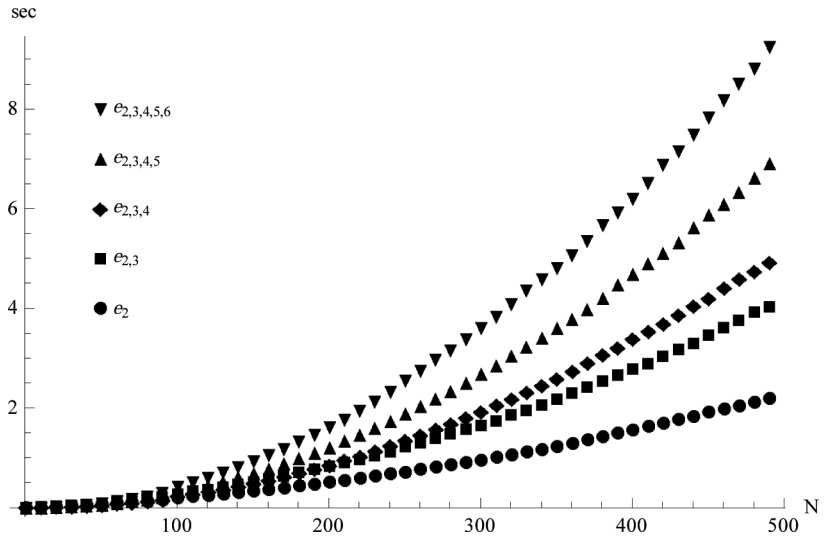

Fig. 2. Computation times for presented algorithm

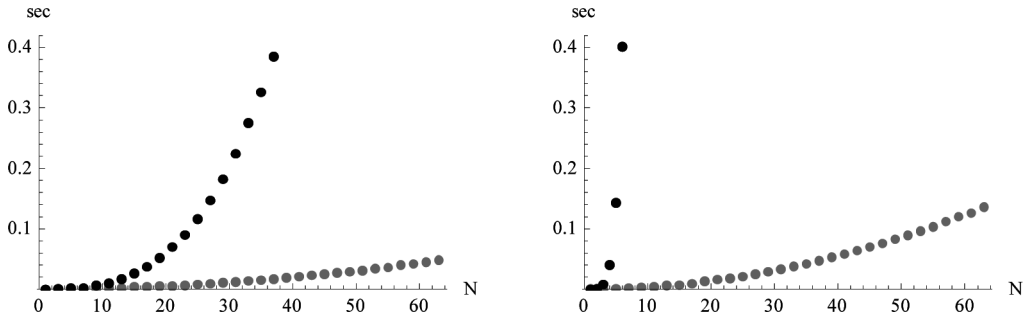

Fig. 3. Comparison of computation times of e_{23} (left) and e_{23456} (rigth). Black dots-standard sum; gray dots–presented algorithm

The hexagonal and square lattices contain $N = 64$ inclusions. The maximal concentrations for the hexagonal and rectangular lattices are $\nu_{max} = \frac{\pi}{\sqrt{12}} \approx 0.9069$ and $\nu_{max} = \frac{\pi}{4} \approx 0.7854$, respectively [9]. The rectangular array contains $9 \times 7 = 63$ inclusions. The maximal concentration for this rectangular array is equal to $\nu_{max} = \frac{7\pi}{36} \approx 0.6109$. The computations were performed for $\nu = 0.6$ with the accuracy $O(\nu^{10})$.

In order to compare the computed sums for different lattices we use the respective error

$$\left| \frac{e_{\text{lattice}_1} - e_{\text{lattice}_2}}{e_{\text{lattice}_1}} \right| < 0.01. \tag{16}$$

Moreover, many terms have to be real (e.g. $e_2 = \pi$, e_{22}, e_{33}, e_{222}, etc). Hence, their imaginary parts display the absolute error. The question which sums have to be real has

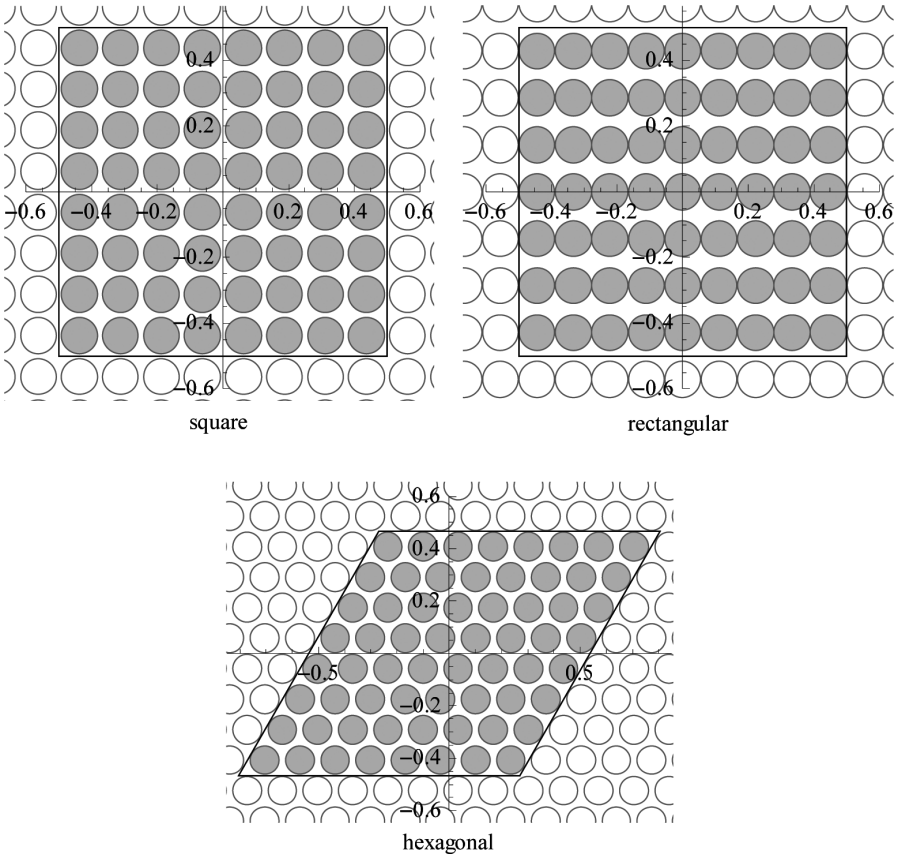

Fig. 4. Considered lattices

been not investigated yet except some sums. Table 2 presents the number of terms errors which exceed a fixed level. Table 3 and Table 4 contain terms errors of which do not exceed 1% with respect to the corresponding terms of the hexagonal lattice ($lattice_1$ in (16)). The criterion (16) can give wrong results for the sums oscillating near zero (e.g. e_{3543}, e_{4532}, e_{23432}, e_{34322} etc). However, there exist few non–zero terms. For instance, the terms $e_{2343222}$, e_{24642}, e_{343332}, $e_{2343222}$, $e_{3432222}$ depend on the initial lattice type. Table 5 and Table 6 include only such terms for which the the error exceeds 10% and the modulus of which is greater than 0.2.

4. Discussion and conclusion

One can consider the set $\{e_{m_1 \ldots m_q}, m_j = 2, 3, \ldots\}$ as a basis in the space of the deterministic or random locations of inclusions. This observation was used in [8] to

create a constructive theory of representative volume elements. The results presented in Tables 3-6 can be considered as the characteristic parameters of the uniform non–overlapping distribution of disks, below denoted as $\mathcal{U}$, in the following way. Let a set of the centres of inclusions be measured in a sample with two–dimensional geometry and the sums $e_{m_1 \ldots m_q}$ are computed for the measured data. If $e_2 \approx \pi$, the considered composite is rather isotropic. This assertion is true at least for not high concentrations. If the rest sums $e_{m_1 \ldots m_q}$ are closed to the values from Tables 3-6, one can assign this composite to the class of composites $\mathcal{U}$ obtained by stirring of the hard inclusions in a host. Let us consider another case when the values $e_{m_1 \ldots m_q}$ coincide with the theoretical values from Tables 3-6 but for higher concentrations than in the sample. This means that the sample could be obtained from a periodic structure by perturbations modelled by random walks in Method II. These perturbations can be restricted, for instance in time. Hence, the hard inclusions are not intimately stirred.

The second interesting question can be stated as follows. Do the final positions of inclusions "remember" the initial locations? Theoretically, the answer must be negative. However, Tables 5-6 demonstrate that at least the terms $e_{2343222}$, e_{24642}, e_{343332}, $e_{2343222}$, $e_{3432222}$ depend on the initial lattice type. This means that the original regular location of inclusions can be restored for composites modelled by random walks (produced by stirring). This observation can be explained by the different scales of convergence of $e_{m_1 \ldots m_q}$ to the limit values when time of random walks tends to infinity. The noted sums converge very slowly to the theoretical values. The number N or time of random walks should be significantly greater for the sums from Tables 5-6 than from Tables 3-4.

The main result of the present paper is a constructive fast algorithm to compute the ER sums for random composites made from collections of non-overlapping, identical, circular disks, embedded in a matrix. The obtained numerical results are applied to the theoretical investigation of the structure of composites and modelling their production by stirring. We have been making experiments to verify our mathematical models the results of which will be published in a separate paper. To the best of our knowledge no such experimental investigations have been carried out.

error	> 0.01	> 0.03	> 0.05	> 0.1	> 0.2
square	81	51	47	37	32
rectangular	96	49	47	35	30

Table 2. Number of terms errors which exceed given value.

sum	hexagonal	square	rectangular
e_2	3.141+0.005 i	3.142	3.141
e_{22}	10.492	10.508	10.497
e_{222}	34.929+0.042 i	35.014	34.961-0.002 i
e_{44}	3.351	3.363	3.382
e_{2222}	119.676	120.119	119.865
e_{55}	-7.581	-7.612	-7.592
e_{2332}	-16.996	-17.077	-17.157
e_{22222}	408.497+0.450 i	410.459+0.023 i	409.400+0.020 i
e_{442}	10.519+0.014 i	10.582-0.006 i	10.615-0.003 i
e_{66}	10.885	10.863	10.853
e_{4422}	36.033+0.007 i	36.293-0.023 i	36.377-0.004 i
e_{2442}	36.883	37.217	37.233
e_{222222}	1421.740	1430.630	1425.990
e_{552}	-23.825-0.048 i	-23.918+0.007 i	-23.841-0.006 i
e_{23322}	-54.970-0.067 i	-55.1976-0.030 i	-55.467+0.011 i
e_{77}	-8.315	-8.379	-8.377
e_{5522}	-82.760-0.045 i	-83.248+0.013 i	-82.847-0.028 i
e_{2552}	-79.019	-79.388	-79.084
e_{3443}	-8.040	-8.111	-8.108
e_{233222}	-196.512+0.100 i	-197.545+0.044 i	-198.195-0.079 i
e_{332222}	-157.040+0.055 i	-157.9080-0.359 i	-158.654+0.326 i
e_{223322}	-191.428	-192.183	-193.053
$e_{2222222}$	4928.980+5.247 i	4966.370+0.552 i	4947.640+0.709 i
e_{662}	34.195+0.042 i	34.118+0.020 i	34.095+0.001 i
e_{24422}	125.254+0.111 i	126.527+0.056 i	126.532+0.016 i
e_{44222}	119.766+0.194 i	120.8410-0.120 i	120.962-0.043 i
e_{88}	6.887	6.905	6.954
e_{6622}	119.789-0.036 i	119.757+0.095 i	119.604+0.086 i
e_{2662}	111.850	111.646	111.584

Tab. 3. Eisenstein-Rayleigh sums errors of which for square and rectangular lattices with respect to hexagonal terms do not exceed 1%

sum	hexagonal	square	rectangular
e_{442222}	417.985+0.203 i	422.3180-0.481 i	422.360-0.076 i
e_{233332}	127.744	127.722	128.796
$e_{22222222}$	17346.200	17506.200	17427.400
e_{772}	-26.137-0.028 i	-26.330-0.035 i	-26.321-0.020 i
e_{25522}	-273.178-0.311 i	-274.8790+0.020 i	-273.447+0.006 i
e_{34432}	-25.255-0.062 i	-25.4490-0.039 i	-25.483+0.021 i
e_{55222}	-275.125-0.504 i	-276.8070-0.046 i	-275.435-0.145 i
$e_{2233222}$	-677.310-1.005 i	-680.6730-0.660 i	-682.763+0.291 i
$e_{2332222}$	-659.282-0.545 i	-662.4020-0.241 i	-664.490-0.311 i
$e_{3322222}$	-536.964-0.684 i	-540.5350-1.495 i	-542.382+1.501 i
e_{99}	-8.252	-8.294	-8.288
e_{6633}	-15.241-0.006 i	-15.324-0.047 i	-15.381+0.020 i
e_{7722}	-93.050+0.032 i	-93.869-0.108 i	-93.743-0.078 i
e_{2772}	-86.915	-87.593	-87.459
e_{4554}	-18.025	-18.055	-18.182
e_{255222}	-932.595+0.140 i	-939.0070+0.301 i	-933.7780+0.166 i
e_{344322}	-82.823-0.039 i	-83.5149-0.116 i	-83.630+0.106 i
e_{552222}	-970.801-0.601 i	-978.6840-0.201 i	-972.521-0.409 i
e_{225522}	-965.793	-973.428	-967.124
$e_{22332222}$	-2366.840-0.319 i	-2378.5100-0.841 i	-2384.320+1.256 i
$e_{23322222}$	-2343.050+1.666 i	-2357.8400+0.455 i	-2361.590-2.169 i
$e_{33222222}$	-1851.620+0.875 i	-1863.1800-4.180 i	-1869.510+5.307 i
$e_{22233222}$	-2485.400	-2501.140	-2504.800
$e_{222222222}$	60806.200+64.308 i	61460.2000+9.809 i	61146.400+13.461 i
e_{882}	21.6135+0.061 i	21.7103-0.015 i	21.8069-0.025 i
e_{26622}	390.301+0.575 i	390.2250-0.031 i	389.901-0.192 i
e_{33552}	20.334-0.053 i	20.297+0.085 i	20.486-0.076 i
e_{66222}	397.879+0.319 i	398.0510+0.404 i	397.460+0.350 i
$e_{2333322}$	407.659+0.328 i	407.0330+0.092 i	410.825-0.357 i

Tab. 4. Continuation of Table 3

term	hexagonal	square	error
e_{3542}	-0.232-0.059 i	-0.177-0.033 i	0.25
e_{4532}	-0.661-0.041 i	-0.559-0.054 i	0.15
e_{23432}	-0.574+0.029 i	-0.983-0.036 i	0.72
e_{34322}	-0.198-0.032 i	-0.459	1.31
e_{3652}	0.398+0.111 i	0.502-0.030 i	0.42
e_{4642}	0.237+0.110 i	0.505-0.002 i	1.11
e_{234322}	-7.523+0.197 i	-8.824-0.054 i	0.18
e_{343222}	0.031-0.043 i	-1.064-0.022 i	20.78
e_{35422}	-0.765-0.195 i	-0.578-0.081 i	0.28
e_{45322}	-2.090-0.226 i	-1.816-0.215 i	0.13
e_{3762}	-0.629+0.060 i	-0.581-0.205 i	0.43
e_{4752}	-0.395-0.126 i	-0.529+0.070 i	0.57
e_{5742}	-2.740-0.136 i	-2.979+0.006 i	0.10
e_{24642}	1.752-0.234 i	2.791+0.041 i	0.61
e_{34443}	0.203-0.086 i	-0.031 i	0.95
e_{333432}	-0.785-0.146 i	-0.255+0.155 i	0.76
e_{343332}	1.642-0.064 i	2.218+0.011 i	0.35
e_{354222}	-5.149-0.714 i	-4.785-0.428 i	0.09
$e_{2234322}$	-41.744-0.869 i	-45.880	0.10
e_{36522}	1.243+0.381 i	1.529-0.151 i	0.46
e_{46422}	0.711+0.426 i	1.693+0.089 i	1.25
$e_{2343222}$	-21.757+0.322 i	-27.078-0.266 i	0.25
$e_{3432222}$	-0.076-0.158 i	-3.414-0.095 i	19.10

Tab. 5. Eisenstein-Rayleigh sums for hexagonal and square lattices.
Last column includes respective error with respect to hexagonal terms

term	hexagonal	rectangular	hex-rect
e_{3542}	-0.232-0.059 i	-0.193-0.073 i	0.17
e_{4532}	-0.661-0.041 i	-0.628-0.009 i	0.07
e_{23432}	-0.574+0.029 i	-1.077-0.127 i	0.92
e_{34322}	-0.198-0.032 i	-0.483+0.118 i	1.61
e_{3652}	0.398+0.111 i	0.536-0.101 i	0.61
e_{4642}	0.237+0.110 i	0.343+0.148 i	0.43
e_{234322}	-7.523+0.197 i	-9.340-0.166 i	0.25
e_{343222}	0.031-0.043 i	-1.224+0.392 i	25.21
e_{35422}	-0.765-0.195 i	-0.604-0.255 i	0.22
e_{45322}	-2.090-0.226 i	-1.938-0.095 i	0.1
e_{3762}	-0.629+0.060 i	-0.585+0.097 i	0.09
e_{4752}	-0.395-0.126 i	-0.410+0.167 i	0.71
e_{5742}	-2.740-0.136 i	-2.813+0.165 i	0.11
e_{24642}	1.752-0.234 i	2.200-0.423 i	0.28
e_{34443}	0.203-0.086 i	0.184+0.241 i	1.48
e_{333432}	-0.785-0.146 i	-0.493-0.189 i	0.37
e_{343332}	1.642-0.064 i	2.104-0.150 i	0.29
e_{354222}	-5.149-0.714 i	-4.687-1.006 i	0.11
$e_{2234322}$	-41.744-0.869 i	-48.079-0.302 i	0.15
e_{36522}	1.243+0.381 i	1.708-0.328 i	0.65
e_{46422}	0.711+0.426 i	1.041+0.486 i	0.41
$e_{2343222}$	-21.757+0.322 i	-29.000-0.661 i	0.34
$e_{3432222}$	-0.076-0.158 i	-4.337+0.982 i	25.23

Tab. 6. Eisenstein-Rayleigh sums for hexagonal and rectangular lattices. Last column includes respective error with respect to hexagonal terms

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Symulacje komórki reprezentacyjnej 2D kompozytu z kołowymi nie nachodzącymi na siebie wtrąceniami

Streszczenie

Rozważmy dwuwymiarowy, dwufazowy okresowy materiał kompozytowy, złożony ze zbioru nienakładających się na siebie identycznych wtrąceń kołowych zanurzonych w osnowie. Zgodnie z teorią komórki reprezentatywnej, efektywna przewodność badanego materiału wyraża się za pomocą uogólnionych sum Eisensteina-Rayleigha (zwanych dalej sumami ER). Bezpośrednie obliczenie sum ER jest możliwe tylko w przypadku sum niższych rzędów. W artykule przedstawiono szybki algorytm obliczający sumy ER wyższych rzędów, opracowany z wykorzystaniem błądzenia losowego oraz metody Monte Carlo. Algorytm ten jest rekurencyjny, tzn. ustalona suma ER

wyrażona jest za pomocą sum niższego rzędu. W celu usprawnienia działania algorytmu wykorzystano algebraiczne zależności między funkcjami Eisensteina i Wieierstrassa oraz między ich pochodnymi. Uzyskane wyniki numeryczne zastosowano do badania struktury materiałów kompozytowych.