

Some computational aspects of iterated structures

Johan Byström^a, Johan Helsing^b, Annette Meidell^{c,*}

^aDepartment of Mathematics, Luleå University of Technology, LTU, SE-97187 Luleå, Sweden

^bDepartment of Solid Mechanics, Royal Institute of Technology, KTH, SE-100 44 Stockholm, Sweden

^cNarvik University College HiN, P.O. Box 385, N-8505 Narvik, Norway

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Abstract

We consider some computational aspects of effective properties for some multi-scale structures. In particular, we discuss iterated square honeycombs and another type of square honeycombs containing up to 4000 small discs randomly distributed inside each square. We present some numerical methods for estimating the effective conductivity with good control of the accuracy. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

By *honeycombs*, one usually means two-dimensional two-component periodic structures where the interior part consists of polygons (typically hexagons or rectangles). *Iterated honeycombs* are, roughly speaking, ‘honeycombs in honeycombs’. Several types of such structures (and also some multi-dimensional generalizations) was studied theoretically by Lukkassen with respect to linear elastic and thermal effective properties in Refs. [17–20]. He found some simple formulae for upper and lower bounds of the corresponding effective parameters. These bounds happen to converge to the same limit as the number of length scales turns to infinity, and it turns out that these limits are optimal. Composite structures of this type are usually referred to as optimal. Other well-known examples are the *Hashin ellipsoidal* structure and the *multi-rank laminate* structure (see Ref. [14]). However, it is important to note that structures, which have the same effective behavior often are different with respect to properties such as local buckling resistance, local and global strength, structural collapse, etc. From this point of view, iterated honeycombs seem to be very interesting, especially because they possess certain suitable symmetry properties (see Ref. [20]).

In this paper, we consider some computational aspects of multi-scale structures of this type. In Sections 2 and 3, we

discuss iterated square honeycombs. In particular, we present a numerical method for estimating the effective conductivity with good control of the accuracy. This method provides a reliable tool for comparing different types of iterated square honeycombs. Up to now, only the case of widely separated length scales has been considered. From a manufacturing point of view, it is interesting to investigate and compare intermediate cases. We therefore also compare some concrete iterated honeycombs.

In Section 4, we consider another type of square honeycombs containing up to 4000 small discs randomly distributed inside each square. Not very long time ago computational problems of this type were considered impossible to solve. It may therefore come as a surprise that we are able to compute the corresponding effective conductivity of such problems, and even with extremely good accuracy. The basis for our numerical estimates is the work of Helsing [12,13] who has developed a fast multi-pole-accelerated iterative scheme for computations of problems with inclusions of arbitrary shape.

Section 5 gives some final comments.

2. Iterated square honeycombs

We start by defining the iterated square honeycomb structure (Fig. 1) by a characteristic function $\chi_{m,k,h}$ (indicator function). Let $0 \leq v \leq 1$, let m, k, h be positive integers and let χ be the characteristic function of the interval $[0, v^{1/(2m)}]$. We define the characteristic function $\chi_{m,k,h}$ on

* Corresponding author.

E-mail address: am@hin.no (A. Meidell).

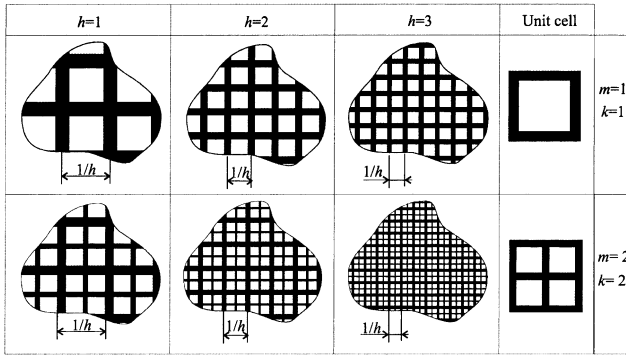


Fig. 1. Iterated square honeycombs.

R^2 as

$$\chi_{m,k,h}(x) = \chi^{(m)}(hx_1)\chi^{(m)}(hx_2),$$

where $\chi^{(m)}$ is found iteratively by letting $\chi^{(i+1)}$ be the $[0,1]$ -periodic extension of the function $\chi^{(i)}(k \cdot v^{1/(2m)} - (1 - v^{1/(2m)})/2)$, $\chi^{(0)} = 1$.

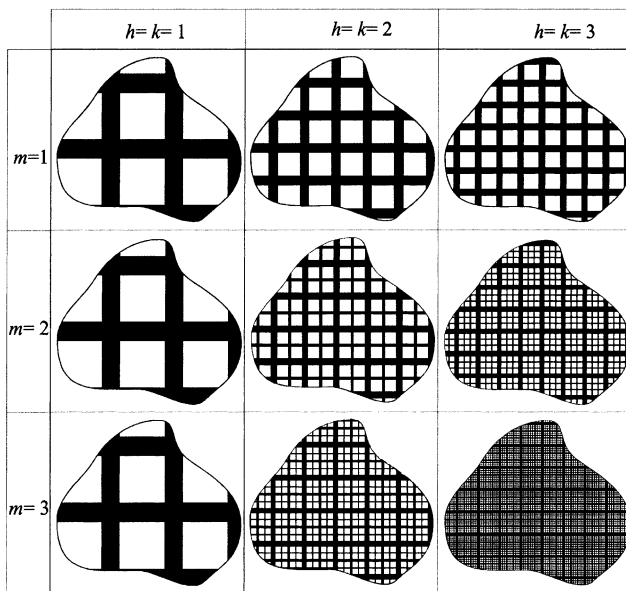
By using this characteristic function, we can define the conductivity $\lambda_{m,k,h}(x)$ as follows:

$$\lambda_{m,k,h}(x) = \lambda_{\text{in}}\chi_{m,k,h}(x) + \lambda_{\text{con}}(1 - \chi_{m,k,h}(x)).$$

Here, λ_{in} and λ_{con} are the conductivities of the interior and the connected part of the iterated square honeycomb-structure, respectively.

In order to be able to speak about effective conductivity for the above structure we consider the following two limit-cases:

- Fix m and k and let h approach infinity. The corresponding effective conductivity is in this case denoted $\lambda_{m,k}$.
- Fix m and let $h = k$ approach infinity (Fig. 2). The corre-

Fig. 2. Iterated square honeycombs for $h = k$.

sponding effective conductivity is in this case denoted $\lambda_{m,\infty}$.

The first of these cases are treated by standard periodic homogenization, i.e. (see Ref. [14])

$$\lambda_{m,k} = \min_{v \in W_{\text{per}}^{1,2}(Y)} \left\{ \frac{1}{|Y|} \int_Y \lambda_{m,k,1}(x) \left(\frac{\partial v}{\partial x_1} + 1 \right)^2 + \lambda_{m,k,1}(x) \times \left(\frac{\partial v}{\partial x_2} \right)^2 dx \right\}, \quad (1)$$

where $Y = [0, 1]^2$, $W_{\text{per}}^{1,2}(Y)$ is the space of Y -periodic functions of the usual Sobolev space $W^{1,2}(Y)$. Moreover, using the well-known property of complementary energy in two-dimensions, see Ref. [14], p. 39, we get the following equivalent variational formula:

$$\frac{1}{\lambda_{m,k}} = \min_{v \in W_{\text{per}}^{1,2}(Y)} \left\{ \frac{1}{|Y|} \int_Y \frac{1}{\lambda_{m,k,1}(x)} \left(\frac{\partial v}{\partial x_1} + 1 \right)^2 + \frac{1}{\lambda_{m,k,1}(x)} \left(\frac{\partial v}{\partial x_2} \right)^2 dx \right\}. \quad (2)$$

In the second case the effective conductivity $\lambda_{m,\infty} = q_m$, where q_m is determined by the following iterative variational formula:

$$q_i = \min_{v \in W_{\text{per}}^{1,2}(Y)} \left\{ \frac{1}{|Y|} \int_Y b_i(x) \left(\frac{\partial v}{\partial x_1} + 1 \right)^2 + b_i(x) \left(\frac{\partial v}{\partial x_2} \right)^2 dx \right\}, \quad (3)$$

$$b_i(x) = q_{i-1}\chi + \lambda_{\text{con}}(1 - \chi), \quad i = 1, \dots, m,$$

$$q_0 = \lambda_{\text{in}}.$$

Similarly as in Eq. (2) we obtain the following equivalent variational formula:

$$\frac{1}{q_i} = \min_{v \in W_{\text{per}}^{1,2}(Y)} \left\{ \frac{1}{|Y|} \int_Y \frac{1}{b_i(x)} \left(\frac{\partial v}{\partial x_1} + 1 \right)^2 + \frac{1}{b_i(x)} \left(\frac{\partial v}{\partial x_2} \right)^2 dx \right\}. \quad (4)$$

Remark 1. The iterative procedure follows by the Iterated Homogenization Theorem of Bensoussan et al. [5]. This theorem is valid for cases when the conductivity $\lambda_{m,h,h}$ is of the form

$$\lambda_{m,h,h}(x) = \lambda(hx, h^2x, \dots, h^m x),$$

where λ is periodic in each variable (which is the case for the honeycombs considered in Refs. [17,20]). In our case, this assumption is slightly modified. However, by mimicking the proof given in Ref. [16] it is not hard to verify that the iterative process remains valid. Moreover, by using the same arguments as in that proof it is also possible to verify

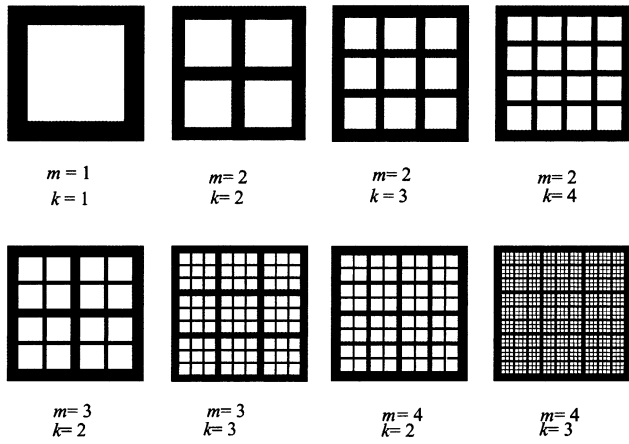


Fig. 3. Example of unit cells for some types of iterated square honeycombs in the case $\nu = 0.52$.

that

$$\lambda_{m,k} \rightarrow \lambda_{m,\infty}$$

as $k \rightarrow \infty$.

For iterated square honeycombs (Fig. 3), the approximation formula of Lukkassen (see Refs. [17,20]) reduces to

$$\frac{1}{\lambda_{m,\infty} - \lambda_{\text{con}}} = \frac{1}{\lambda_{\text{in}} - \lambda_{\text{con}}} \frac{1}{\nu} + \frac{r_m}{1 + \nu^{1/(2m)}} \frac{1 - \nu}{\lambda_{\text{con}} \nu}, \quad (5)$$

where $\nu^{1/(2m)} \leq r_m \leq 1$ (in fact, this formula is also valid for iterated hexagonal honeycombs, see Ref. [18]). Note that Eq. (5) yields the convergence

$$\lambda_{m,\infty} \rightarrow \lambda_{\infty,\infty} = \lambda_{\text{con}} + \left(\frac{1}{\lambda_{\text{in}} - \lambda_{\text{con}}} \frac{1}{\nu} + \frac{1 - \nu}{2\lambda_{\text{con}} \nu} \right)^{-1}, \quad (6)$$

as $m \rightarrow \infty$, which is precisely the Hashin–Shtrikman upper bound for $\lambda_{\text{in}} < \lambda_{\text{con}}$ and the Hashin–Shtrikman lower bound if $\lambda_{\text{in}} > \lambda_{\text{con}}$. We recall that the Hashin–Shtrikman bounds are the best possible within the class of macroscopically isotropic structures (for the original proof, see Ref. [11]).

3. Numerical computations of effective properties for iterated square honeycombs

In this section, we study numerical computations of the effective conductivities $\lambda_{m,k}$ and $\lambda_{m,\infty}$. The method for our numerical estimations is based on replacing $W_{\text{per}}^{1,2}(Y)$ with a finite dimensional subset of $W_{\text{per}}^{1,2}(Y)$ in Eqs. (1), (2) and (3), (4), respectively. In this way we obtain upper and lower numerical estimates $\lambda_{m,k}^+$ and $\lambda_{m,k}^-$ for $\lambda_{m,k}$. In particular, we obtain upper and lower numerical estimates $\lambda_{m,\infty}^+$ and $\lambda_{m,\infty}^-$ for $\lambda_{m,\infty}$ which are found iteratively by replacing $q_i(x)$ with $q_i^+(x)$ and $q_i^-(x)$ in Eqs. (3) and (4), respectively. We note that the geometry of the problem is the same on each step. Based on this geometry, we can create a fixed FEM-

mesh (with finest mesh-refinement in the corners) which we can use on all the $2m$ steps. As an approximation for $\lambda_{m,k}$ we use the number $\tilde{\lambda}_{m,k}$

$$\tilde{\lambda}_{m,k} = 1/2(\lambda_{m,k}^- + \lambda_{m,k}^+),$$

and let $r_{m,k}$ denote the corresponding maximum possible relative numerical error estimate (in %) i.e.

$$r_{m,k} = 100 \frac{\lambda_{m,k}^+ - \lambda_{m,k}^-}{\lambda_{m,k}^+ + \lambda_{m,k}^-}.$$

Moreover, let $d_{m,k}$ denote the deviation between $\lambda_{m,k}$ and $\lambda_{\infty,\infty}$ (in %) i.e.

$$d_{m,k} = 100 \frac{\lambda_{\infty,\infty} - \lambda_{m,k}}{\lambda_{m,k}} \quad (7)$$

and let $\tilde{d}_{m,k}$ denote the approximate deviation between $\tilde{\lambda}_{m,k}$ and $\lambda_{\infty,\infty}$ (in %), i.e.

$$\tilde{d}_{m,k} = 100 \frac{\lambda_{\infty,\infty} - \tilde{\lambda}_{m,k}}{\tilde{\lambda}_{m,k}}$$

(with maximum possible numerical error less than $r_{m,k}(\lambda_{\infty,\infty}/\lambda_{m,k}^+)$). If the maximum error estimate is too large, we have to refine the mesh even more and start all over again with performing another $2m$ computations.

In the case $k < \infty$, we only have to perform two computations instead of $2m$. Here, $\lambda_{m,k}^+$ and $\lambda_{m,k}^-$ are found directly from Eqs. (1) and (2). However, when k is large the problem becomes strongly non-homogeneous and in order to obtain an accurate approximation we will need an enormous amount of finite elements. We have performed a number of numerical calculations. In Fig. 4 (see also Appendix A) we present some of the exact plots of $d_{m,k}$ (actually of $\tilde{d}_{m,k}$ but the difference is insignificant) as a function of the area-fraction ν for some values of m and k . Each plot is for the extreme case $\lambda_{\text{in}}/\lambda_{\text{con}} \approx 0$ (for which $d_{m,k}$ is assumed to be largest possible, cf. Refs. [21,23]).

By evaluating $\lambda_{m,\infty}$ from the formula of Lukkassen (5) with $r_m = 1$ and replacing $\lambda_{m,k}$ in Eq. (7) with this value we

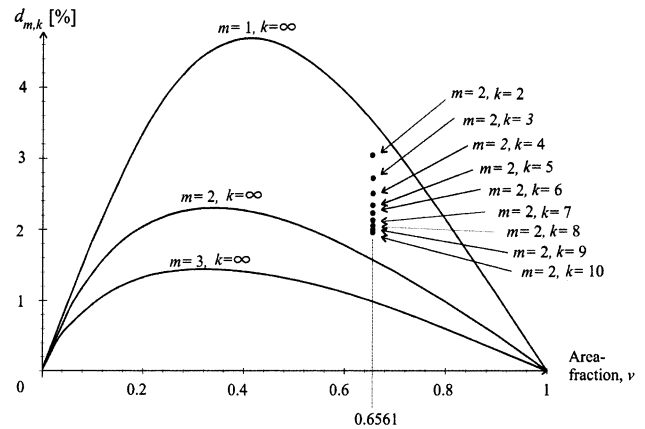


Fig. 4. Difference between the effective conductivity and the Hashin–Shtrikman upper bound.

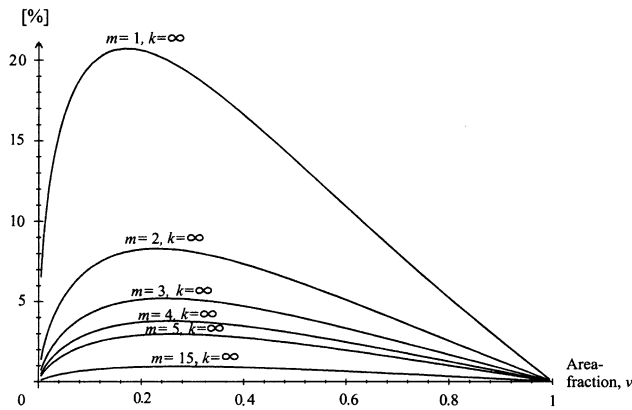


Fig. 5. Upper bound for $d_{m,\infty}$ according to the approximation formula of Lukkassen.

obviously obtain an upper bound for $d_{m,k}$. In order to compare with our numerical calculations we have plotted this upper bound for some values of m in Fig. 5.

Let us give a few comments to the numerical results. It seems that for a fixed value of m the conductivity increases with k . However, the convergence, as k goes to ∞ , is slower than we expected (see Fig. 4). From a manufacturing point of view, it is obvious that the number of white squares $k^{2(m-1)}$ in each unit cell is an important parameter (it is easier to manufacture a structure with few large squares than many small ones). We observe from Table A2 in Appendix A that the conductivity may not necessarily increase with the number $k^{2(m-1)}$ (compare the case $m=2$, $k=8$ with the case $m=3$, $k=3$). However, due to the error estimates (see Table A2 in the Appendix A), we cannot draw any firm conclusions on this matter for the computed cases. For large values of k this fact is obvious from the $k=\infty$ -curves in Fig. 4, and the convergence result [6].

4. Square honeycombs with highly inhomogeneous squares

By using standard finite element method programs the accuracy of the computations when $k=\infty$ is sufficient for the purpose of comparison. The computations for finite values of k are less accurate (see the table values in Appendix A). When the unit cell consists of more than around 100 objects (in this case squares) it turns out to be almost impossible to obtain useful results by standard finite element method programs.

Now, consider the case when the collection of squares is replaced with a much larger collection of randomly distributed disks. There are recently developed methods [9,13] that are capable of rapidly solving very complex cell structures to high accuracy. In order to illustrate, we will here use an integral equation based adaptive scheme developed by Helsing [12,13] and accelerated with the fast multi-pole method [10]. We will use this scheme to compute the

effective properties of pseudorandom structures with 1024 and 4096 inclusions in the corresponding cells.

The pseudorandom disk configurations were generated by a Monte Carlo procedure of Metropolis type [24]. We begin by placing all disks at the lattice points of a regular square array. Each disk is then given a small tentative displacement in a random direction. The displacement is accepted or rejected according to whether or not the new position will cause the disk to overlap its neighbors. One iteration step consists of trying to move each disk once so that the ratio of moved disks to the total number of disks is about one half. This process is iterated several times until equilibrium is achieved. The random configurations we use in our examples were generated using thousands of iteration steps.

In our example the geometries consist of either 1024 or 4096 randomly placed disks with centers in a square of size 0.8×0.8 . All disks are of the same size and chosen such that the total area fraction of the disks is 0.6. The disks have conductivity 1000 and the surrounding matrix has conductivity 1. Finally this square is then itself placed in a square of size 1.0×1.0 , see Fig. 6.

The cell problem is then solved on these unit cells with periodic boundary conditions and the homogenized conductivity is computed. This procedure is executed for five different realizations of the cell structure. Four structures contain 1024 disks and one structure contains 4096 disks. The relative error for the conductivities in the 1024 disk computations is estimated to be 10^{-9} and the relative error for the conductivity in the 4096 disk computation is estimated to be 10^{-7} . The mean value and maximum deviation for all five configurations are then computed to give the range of the homogenized conductivity.

We compare the conductivity of the two-scale cell structure with that of a cell where the square with disks is replaced with a square with a homogeneous material with

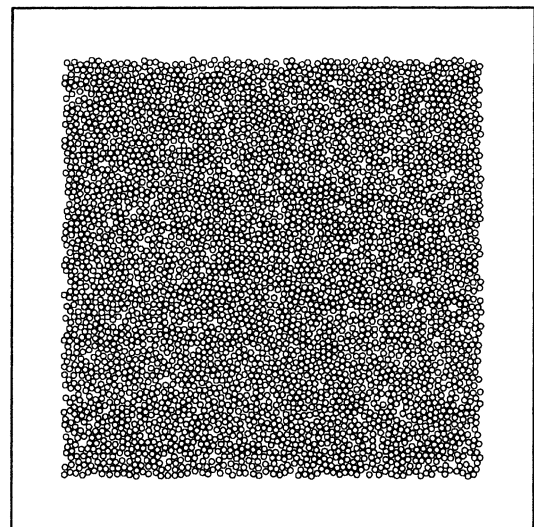


Fig. 6. Unit cell of square honeycomb containing 4096 disks. The effective conductivity in the x -direction is estimated to 2.5392653.

the same effective properties as the square with disks. The squares with disk inclusions have conductivities equal to

$$5.13 \pm 0.07, \quad (8)$$

and the corresponding two-scale structures with these squares included in the larger square have conductivities of

$$2.53 \pm 0.02. \quad (9)$$

By replacing the included square consisting of disks with a square consisting of a homogeneous material with effective conductivity equal to 5.13, we obtain a conductivity equal to 2.53, which is within the estimates given in Eq. (9). This agreement suggests that it is admissible to replace the underlying heterogeneous scale by a homogeneous one, which was expected.

One might think that the value in Eq. (8) in the random case is close to the effective conductivity of a periodic distribution of such disks. However, it turns out that the conductivities are 15–22% lower in the periodic case, being 4.322 for square packing and 4.011 for hexagonal packing. This shows that percolation effects in the random case considerably affects the conductivities for this volume fraction of 0.6.

5. Some final comments

The theoretical work on iterated honeycombs performed in Refs. [17–20] was later followed by studies of some non-linear properties (see Refs. [6,17,28,29]). In particular, in Ref. [6] it was observed that the macroscopic behavior of reiterated honeycombs may be more extreme than that of the best possible *laminates of rank 2*. This is an interesting observation since for linear problems rank 2-laminates have proven to be best possible within the class of two-component structures. In all these studies non-linear versions of The Iterated Homogenization Theorem has played an essential role. For the most general non-linear versions we refer to Refs. [6,15,16]. An anisotropic version of the formula of Lukkassen corresponding to an infinite number of iteration levels was compared with the effective properties of rectangular honeycombs in Refs. [22,23]. Here, a surprisingly good agreement was observed between the numerical calculations and this formula.

Concerning the Iterated Homogenization Theorem for linear problems including elasticity we refer to Ref. [2]. See also Ref. [1] for a different approach by use of so-called multi-scale convergence. There are many other examples in the literature where iterated homogenization are used. For iterated laminates, we refer to Francfort and Murat [8], Milton [25,26], Avellaneda et al., [3,4] and the references given there. There is also a new class of optimal microstructure found recently, see Ref. [27].

To get satisfactory effective conductivities for certain types of random media, one has to solve cell problems

with thousands of random inclusions. This is a task that is extremely hard with standard type of software for numerical solution of partial differential equations, such as the finite element method programs. The calculations performed in Section 4 indicates that the method developed in Ref. [12,13] is a powerful tool.

Reiterated homogenization can be used to solve many practical problems. We here refer to Ref. [7] where reiterated homogenization was used to compute the elastic properties of woven composites.

Appendix A

The numerical values for the computations of the solid lines in Fig. 4 are presented in Table A1.

In Table A2, we present the numerical values for the computations of points in Fig. 4.

Table A1

v	$\tilde{\lambda}_{m,k}$	Max error ^a	$r_{m,k}$ (%)	$\tilde{d}_{m,k}$ (%)
$m = 1$				
0.9	0.05206404	0.920×10^{-5}	0.18×10^{-1}	1.09
0.8	0.1087817	0.175×10^{-4}	0.16×10^{-1}	2.14
0.7	0.1711508	0.213×10^{-4}	0.12×10^{-1}	3.11
0.6	0.2405497	0.291×10^{-4}	0.12×10^{-1}	3.93
0.5	0.3189800	0.372×10^{-4}	0.12×10^{-1}	4.50
0.4	0.4094063	0.486×10^{-4}	0.12×10^{-1}	4.68
0.3	0.5161171	0.500×10^{-4}	0.97×10^{-2}	4.33
0.25	0.5773503	0.600×10^{-4}	0.10×10^{-1}	3.92
0.2	0.6449768	0.810×10^{-4}	0.13×10^{-1}	3.36
0.1	0.8034062	0.628×10^{-4}	0.78×10^{-2}	1.84
0.05	0.8963494	0.654×10^{-4}	0.73×10^{-2}	0.94
$m = 2$				
0.9	0.05236119	0.130×10^{-4}	0.25×10^{-1}	0.52
0.8	0.1100282	0.245×10^{-4}	0.22×10^{-1}	0.98
0.7	0.1740242	0.216×10^{-4}	0.12×10^{-1}	1.41
0.6	0.2456425	0.227×10^{-4}	0.92×10^{-2}	1.77
0.5	0.3265793	0.285×10^{-4}	0.87×10^{-2}	2.07
0.4	0.4191237	0.333×10^{-4}	0.80×10^{-2}	2.25
0.3	0.5264710	0.348×10^{-4}	0.66×10^{-2}	2.28
0.25	0.5870526	0.297×10^{-4}	0.51×10^{-2}	2.20
0.2	0.6533343	0.408×10^{-4}	0.62×10^{-2}	2.04
0.1	0.8070581	0.243×10^{-4}	0.30×10^{-2}	1.38
0.05	0.8975459	0.203×10^{-4}	0.23×10^{-2}	0.80
$m = 3$				
0.9	0.05245739	0.111×10^{-4}	0.21×10^{-1}	0.33
0.8	0.1104148	0.255×10^{-4}	0.23×10^{-1}	0.63
0.7	0.1749115	0.241×10^{-4}	0.14×10^{-1}	0.89
0.6	0.2472525	0.258×10^{-4}	0.11×10^{-1}	1.11
0.5	0.3290854	0.273×10^{-4}	0.83×10^{-2}	1.29
0.4	0.4226275	0.281×10^{-4}	0.66×10^{-2}	1.41
0.3	0.5308423	0.303×10^{-4}	0.57×10^{-2}	1.44
0.25	0.5917019	0.263×10^{-4}	0.44×10^{-2}	1.40
0.2	0.6579456	0.292×10^{-4}	0.44×10^{-2}	1.33
0.1	0.8103420	0.206×10^{-4}	0.25×10^{-2}	0.97
0.05	0.8992316	0.125×10^{-4}	0.14×10^{-2}	0.62

^a $(\lambda_{m,k}^+ - \lambda_{m,k}^-)/2$.

Table A2

	m	k	NOS ^a	$\tilde{\lambda}_{m,k}$	$r_{m,k}$ (%)	$\tilde{d}_{m,k}$
Volume-fraction (0.81) ² = 0.6561	2	1	1	0.200650	4×10^{-5}	3.4919
	2	2	4	0.201534	1.6×10^{-4}	3.0380
	2	3	9	0.202145	1.6×10^{-4}	2.7265
	2	4	16	0.202582	3.7×10^{-4}	2.5049
	2	5	25	0.202892	2.1×10^{-4}	2.3483
	2	6	36	0.203147	2.6×10^{-4}	2.2198
	2	7	49	0.20333	6.6×10^{-4}	2.1278
	2	8	64	0.20348	5.7×10^{-4}	2.0526
	2	9	81	0.20358	6.3×10^{-4}	2.0024
	2	10	100	0.20367	6.0×10^{-4}	1.9574
	2	∞	∞	0.204436	2.9×10^{-5}	1.5753
	3	2	16	0.202284	3.7×10^{-4}	2.6559
	3	3	81	0.20322	6.1×10^{-4}	2.1831
	3	∞	∞	0.205615	2.0×10^{-5}	0.9929
	4	2	64	0.202945	6.3×10^{-4}	2.3216

^a Number of squares in the unit cell.

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