Effective properties of composites with unidirectional cylindrical fibers

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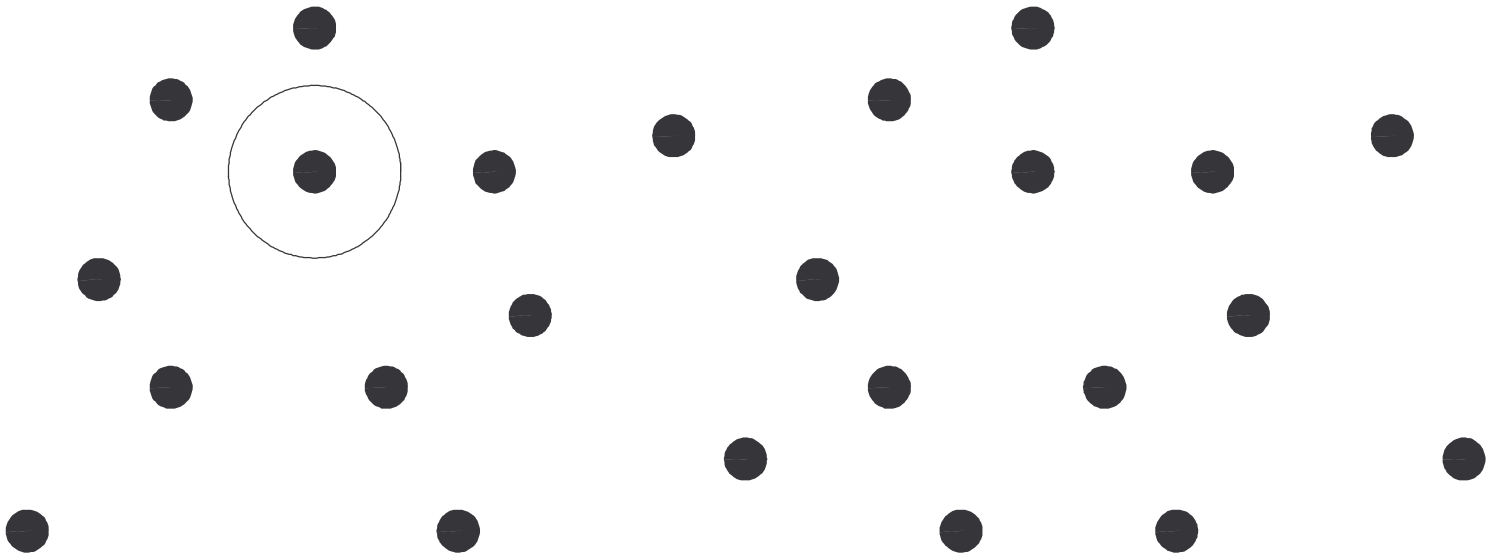
Main presented result:

An effective algorithm is constructed to calculate the effective conductivity of the composites with many different circular inclusions in the unit cell. The final formula for the effective conductivity tensor involves locations of the centers of inclusions, conductivities of constitutes and radii of inclusions in analytical form.

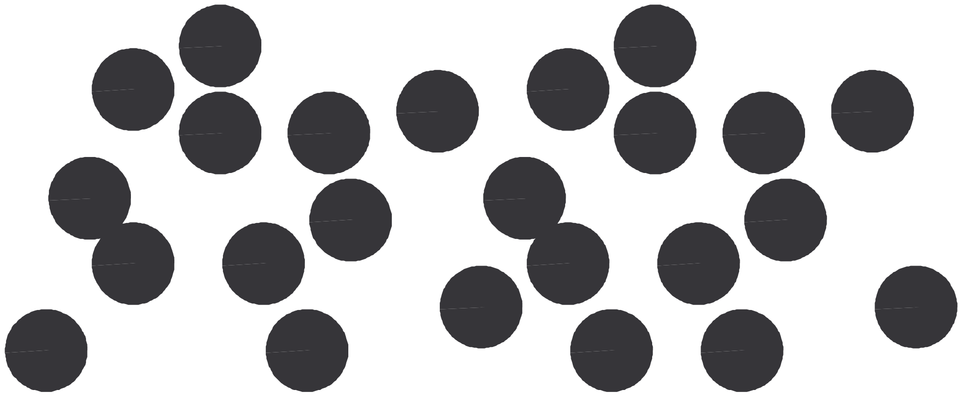
Clausius-Mossotti (Maxwell-Garnett) approximation $\lambda_e \approx \frac{1+\rho v}{1-\rho v}$,

whrere v is the concentration, $\rho = \frac{\lambda^- - 1}{\lambda^- + 1}$ is a contrast parameter.



1. Statement of the problem

Geometry:



Equations: $\Delta u = 0$ (Laplace equation)

Conjugation conditions: $u^+ = u^-$, $\lambda^+ \frac{\partial u^+}{\partial n} = \lambda^- \frac{\partial u^-}{\partial n}$ on the boundary of inclusions ($\lambda^+ = 1$)

Introduce complex potentials: $u(z) = \mathrm{Re}(\phi(z))$ in matrix

$u(z) = \frac{2}{1+\lambda^-} \mathrm{Re}\, \phi_k(z)$ in the k-th inclusion

Write the conjugation conditions in terms of the complex potentials

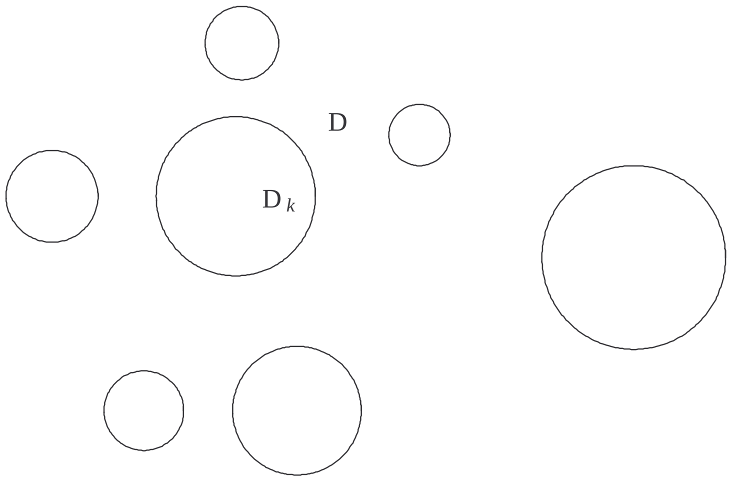
$$\phi(t) = \phi_k(t) - \rho\, \overline{\phi_k(t)}, \quad |\, t - a_k \,| = r_k, \; k = 1, 2, \; ..., n \qquad (1.1)$$

<u>Note.</u> General representation of the function harmonic in multiply connected domain

$$u(z) = \mathrm{Re}(\phi(z) + \sum_{k=1}^{n} A_k \ln(z - a_k)), \text{ where } A_k \in \mathbb{R} \text{ and } \sum_{k=1}^{n} A_k = 0. \qquad (1.2)$$

2. Riemann-Hilbert problems for multiply connected domains

Consider mutually disjointed disks $D_k = \{z \in \mathbb{C}: |z - a_k| < r_k\}$, $k = 1, 2, ..., n$, in the complex plane $\mathbb{C}$, $D = \mathbb{C} \setminus \bigcup_{k=1}^{n} \overline{D_k}$. Given $\lambda(t)$, $f(t)$ as Hölder continuous functions on ∂D_k.



Find a function ϕ(t) analytic in D continuous in $D \bigcup \partial D$ with the following boundary condition

$$\mathrm{Re}\,\overline{\lambda(t)}\,\phi(t) = f(t) \text{ on } |t - a_k| = r_k,\ k = 1, 2, ..., n. \qquad (2.1)$$

This problem has been discussed in classical books [Gakhov, Muskhelishvili, Vekua]. One can find there the solution of (2.1) in closed form for simple and double connected domains ($n = 1$ or $n = 2$).

Complete solution of the scalar problem (2.1) is obtained in analytic form. The problem (2.1) is closely related to harmonic measures of the domain D, the classical Dirichlet and Neumann problems, mixed problems, the Schwarz operator and so forth.

Functional equations

The crucial points in solution to the problem (2.1) is to reduce them to functional equations. The simplest functional equation has the form

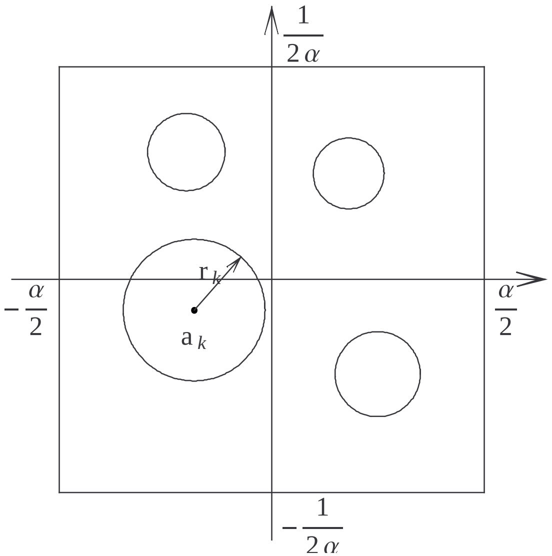
$$\phi(z) = \phi[\alpha(z)] + g(z), \quad |z| \leq r, \qquad (2.2)$$

where known function $g(z)$ and unknown function $\phi(z)$ are meromorphic in $|z| < r$ and continuous in $|z| \leq r$. The given function $\alpha(z)$ maps conformally $|z| \leq r$ into $|z| < r$; $\alpha(z_0) = z_0$; $g(z_0) = 0$.

Equation (2.2) is solved by the method of sucessive approximations: $\phi(z) = \sum_{k=0}^{\infty} g[\alpha^k(z)] + \text{constant}$.

3. Boundary value problems in a class of periodic functions and functional equations

Representative cell:



Conjugation conditions: $u^+ = u^-$, $\lambda^+ \frac{\partial u^+}{\partial n} = \lambda^- \frac{\partial u^-}{\partial n}$ on the boundary of inclusions ($\lambda^+ = 1$)

Quasi-periodicity conditions: $u(z+\alpha) = u(z) + \alpha$, $u(z + 1/i\alpha) = u(z)$. External field is applied in the x-direction.

<u>Note.</u> General representation of the doubly periodic function harmonic in multiply connected domain

$u(z) = \mathrm{Re}(\phi(z) + \sum_{k=1}^{n} A_k(\sigma(z-a_k) + a_k\,\zeta(z-a_k)))$, where $A_k \in \mathbb{R}$ and $\sum_{k=1}^{n} A_k = 0$; $\sigma(z)$ and $\zeta(z)$ are Weierstrass's functions (compare to (1.2)).

$\mathbb{R}$- linear problem in a class of doubly periodic functions:

$$\phi(t) = \phi_k(t) - \rho_k \overline{\phi_k(t)}, \quad |t - a_k| = r_k, \ k = 1, 2, \ldots, n. \tag{3.1}$$

The $\mathbb{R}$- linear problem (3.1) for the square array ($\alpha = 1$) is reduced to the functional equations

$$\psi_m(z) = \sum_{k=1}^{n} \rho_k \sum_{m_1, m_2}{}' \left(\frac{r_k}{z - a_k - \alpha m_1 - i\alpha^{-1} m_2}\right)^2 \overline{\psi_k\left(\frac{r_k{}^2}{\overline{z - a_k - \alpha m_1 - i\alpha^{-1} m_2}} + a_k\right)} + 1,$$

$$|z - a_m| \leq r_m, \ m = 1, 2, \ldots, n. \tag{3.2}$$

Consider (3.2) in the Banach $\mathcal{B}$ space of functions $\Psi(z) = \psi_m(z)$ analytic in each disk $|z - a_m| < r_m$ and continuous in $|z - a_m| \leq r_m$ ($m = 1, 2, \ldots, n$) with the norm $||\Psi|| = \max_{1 \leq m \leq n} \max_{|z - a_m| \leq r_m} |\psi_m(z)|$.

Theorem 1. Equation (3.2) has a unique solution in $\mathcal{B}$. This solution can be found by the method of successive approximations.

Constructive solution to functional equations (3.2):

Fix $k \neq m$. $\psi_k(z) = \sum_{s=1}^{\infty} \psi_{ks}(z - a_k)^s$ – Taylor series

$$\sum_{m_1, m_2} \left(\frac{r_k}{z - a_k - \alpha m_1 - i \alpha^{-1} m_2}\right)^2 \overline{\psi_k\left(\frac{r_k{}^2}{\overline{z - a_k - \alpha m_1 - i \alpha^{-1} m_2}} + a_k\right)} =$$

$$\sum_{m_1, m_2} \left(\frac{r_k}{z - a_k - \alpha m_1 - i \alpha^{-1} m_2}\right)^2 \overline{\sum_{s=1}^{\infty} \psi_{ks} \left(\frac{r_k{}^2}{\overline{z - a_k - \alpha m_1 - i \alpha^{-1} m_2}}\right)^s} =$$

$$\sum_{s=1}^{\infty} \overline{\psi_{ks}}\, r_k{}^{2(s+1)} \sum_{m_1, m_2} \left(z - a_k - \alpha m_1 - i\alpha^{-1} m_2\right)^{-(s+2)} = \sum_{s=1}^{\infty} \overline{\psi_{ks}}\, r_k{}^{2(s+1)} E_{s+2}(z - a_k)$$

4. Eisenstein-Rayleigh lattice sums and Eisenstein functions

Eisenstein summation (see A. Weil, Elliptic Functions According to Eisenstein and Kronecker. Berlin: Springer -Verlag (1976))

$$\sum_{m_1,\, m_2 \in \mathbb{Z}} := \lim_{M\to\infty} \lim_{N\to\infty} \sum_{m_2=-M}^{M} \sum_{m_1=-N}^{N}$$

Consider the lattice sums

$$S_{2k} = \sum_{m_1,\, m_2}{}^{/} \frac{1}{(\alpha m_1 + i\,\alpha^{-1} m_2)^{2k}}, \qquad k = 1, 2, \ldots \tag{4.1}$$

introduced by Eisenstein (1849) and by Rayleigh (1892).

$$S_2 = \left(\frac{\pi}{\alpha}\right)^2 \left(\frac{1}{3} - 8 \sum_{s=1}^{\infty} \frac{m\, h^{2m}}{1-h^{2m}}\right), \qquad \text{where } h = \exp\left(-\frac{\pi}{\alpha^2}\right),$$

$$S_4 = \frac{1}{3} \left(\frac{\pi}{\alpha}\right)^4 \left(\frac{1}{15} + 16 \sum_{s=1}^{\infty} \frac{m^3\, h^{2m}}{1-h^{2m}}\right),$$

$$S_6 = \frac{1}{15} \left(\frac{\pi}{\alpha}\right)^6 \left(\frac{2}{63} - 16 \sum_{s=1}^{\infty} \frac{m^5\, h^{2m}}{1-h^{2m}}\right),$$

$$S_{2k} = \frac{3}{(2k+1)(2k-1)(k-3)} \sum_{m=2}^{k-2} (2m-1)(2k-2m-1) S_{2m} S_{2(k-m)}, \quad k = 4, 5, \ldots$$

For the square array ($\alpha = 1$) we have $S_2 = \pi$.

Eisenstein functions:

$$E_k(z) = \sum_{m_1, m_2} \frac{1}{\left(z - \alpha m_1 - i\, \alpha^{-1} m_2\right)^k}, \quad k = 1, 2, 3, \ \ldots$$

Constructive formulas:

$$E_1(z) = \zeta(z) - S_2\, z, \quad E_2(z) = \wp(z) + S_2, \quad E_{k+1}(z) = -\frac{1}{k}\, E_k{}'(z), \ \ k = 2, 3, \ \ldots,$$

where $\zeta(z)$ and $\wp(z)$ are Weierstrass's functions.

Theorem 2. Let $\psi_k(z)$ be a solution of functional equations (3.2) in the case $\rho_k = \rho, \ r_k = r$. Then it admits the representation

$$\psi_k(z) = \sum_{q=0}^{\infty} \psi_k^{(q)}(z)\, r^{2q}, \qquad (4.2)$$

$$\psi_m^{(0)}(z) = 1, \qquad \psi_m^{(q+1)}(z) = \rho \sum_{k=1}^{n} \left(\overline{\psi_{0\,k}^{(q)}}\, E_2{}^*(z - a_k) + \overline{\psi_{1\,m}^{(q-1)}}\, E_3{}^*(z - a_k) + \ldots + \overline{\psi_{q,k}^{(0)}}\, E_{q+2}{}^*(z - a_k) \right),$$

$$k = 1, 2, \ \ldots, n; \ \ q = 0, 1, \ \ldots. \qquad (4.3)$$

Here $\psi_{j\,k}^{(q)}$ is the j –th coefficient of the Taylor expansion of $\psi_k^{(q)}(z)$. The series (4.2) converges uniformly in the closure of D_k.

Here $E_p{}^*(z - a_k) := E_p(z - a_k)$, if $k \neq m$; $E_p{}^*(z - a_k) := E_p(z - a_k) - \frac{1}{(z - a_k)^p}$, if $k = m$.

5. Effective conductivity tensor $\Lambda_e = \begin{pmatrix} \lambda_e^x & \lambda_e^{xy} \\ \lambda_e^{xy} & \lambda_e^y \end{pmatrix}$

$$\lambda_e^x - i\lambda_e^{xy} = 1 + 2\sum_{k=1}^{n} \rho_k v_k \psi_k(a_k),$$

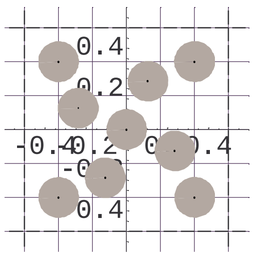
where $v_k = \pi r_k^2$ is the area fraction of the inclusion of conductivity λ_k. Introduce the values

$$\mathbb{X}[p_1 \ldots p_M] = \sum_{m,k_0,\ldots,k_M}^{n} E_{p_1}(a_m - a_{k_1})\overline{E_{p_2}(a_{k_1} - a_{k_2})} \ldots C^{M-1} E_{p_M}(a_{k_{M-1}} - a_{k_M}),$$

where C^{M-1} – is the operator of complex conjugation.

Consider the case of identical inclusions ($\rho_k = \rho$, $r_k = r$) and macroscopically isotropic composites. Then

$$\lambda_e = 1 + 2\rho v \sum_{p=1}^{\infty} A[\![p]\!] v^{p-1}$$



$$A[\![2]\!] = \frac{\rho}{\pi\, n^2}\, \mathbb{X}[2]$$

$$1.\ \rho$$

$$A[\![3]\!] = \frac{\rho^2}{\pi^2\, n^3}\, \mathbb{X}[2, 2]$$

$$2.31326\, \rho^2$$

$$A[\![4]\!] = \frac{1}{\pi^3\, n^4}\, \left(-2\, \rho^2\, \mathbb{X}[3, 3] + \rho^3\, \mathbb{X}[2, 2, 2]\right)$$

$$1.02069\, \rho^2 + 3.62652\, \rho^3$$

$$A[\![5]\!] = \frac{1}{\pi^4\, n^5}\, \left(6\, \rho^2\, \mathbb{X}[4, 4] - 2\, \rho^3\, (\mathbb{X}[3, 3, 2] + \mathbb{X}[2, 3, 3]) + \rho^4\, \mathbb{X}[2, 2, 2, 2]\right)$$

$$4.21634\, \rho^2 - 2.04138\, \rho^3 + 8.24068\, \rho^4$$

$$A[\![6]\!] = \frac{1}{\pi^5\, n^6}\, \left(-24\, \rho^2\, \mathbb{X}[5, 5] + 6\, \rho^3\, (\mathbb{X}[4, 4, 2] + \mathbb{X}[3, 4, 3] + \mathbb{X}[2, 4, 4]) - 2\, \rho^4\, (\mathbb{X}[3, 3, 2, 2] + \mathbb{X}[2, 3, 3, 2] + \mathbb{X}[2, 2, 3, 3]) + \rho^5\, \mathbb{X}[2, 2, 2, 2, 2]\right)$$

$$7.73167\, \rho^2 + 8.43267\, \rho^3 + 7.24832\, \rho^4 + 14.5795\, \rho^5$$

$$A[\![7]\!] = \frac{1}{\pi^6\, n^7}\, \Big(120\, \rho^2\, \mathbb{X}[6, 6] - 24\, \rho^3\, (\mathbb{X}[2, 5, 5] + \mathbb{X}[3, 5, 4] + \mathbb{X}[4, 5, 3] + \mathbb{X}[5, 5, 2]) +$$
$$6\, \rho^4\, (\mathbb{X}[2, 2, 4, 4] + \mathbb{X}[2, 3, 4, 3] + \mathbb{X}[3, 3, 3, 3] + \mathbb{X}[2, 4, 4, 2] + \mathbb{X}[3, 4, 3, 2] + \mathbb{X}[4, 4, 2, 2]) -$$
$$24\, \rho^5\, (\mathbb{X}[2, 2, 2, 3, 3] + \mathbb{X}[2, 2, 3, 3, 2] + \mathbb{X}[2, 3, 3, 2, 2] + \mathbb{X}[3, 3, 2, 2, 2]) + \rho^6\, \mathbb{X}[2, 2, 2, 2, 2]\Big)$$

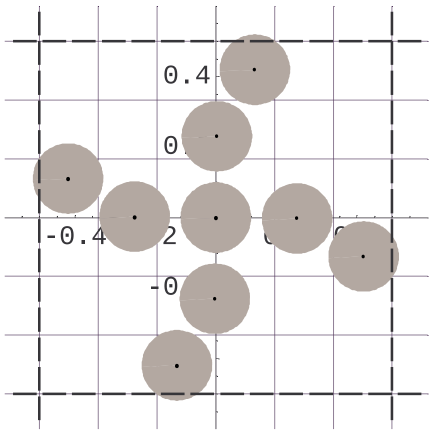
$$7.15993\, \rho^2 + 15.4633\, \rho^3 + 33.1164\, \rho^4 + 181.633\, \rho^5 + 31.1353\, \rho^6$$

$$\lambda_e = 1 + 2\, v\, \rho + 2.\, v^2 \rho^2 + 4.62652\, v^3 \rho^3 + v^4 (2.04138\, \rho^3 + 7.25304\, \rho^4) + v^5 (8.43267\, \rho^3 - 4.08276\, \rho^4 + 16.4814\, \rho^5) + v^6 (15.4633\, \rho^3 + 16.8653\, \rho^4 + 14.4966\, \rho^5 + 29.159\, \rho^6) + v^7 (14.3199\, \rho^3 + 30.9267\, \rho^4 + 66.2327\, \rho^5 + 363.267\, \rho^6 + 62.2707\, \rho^7)$$

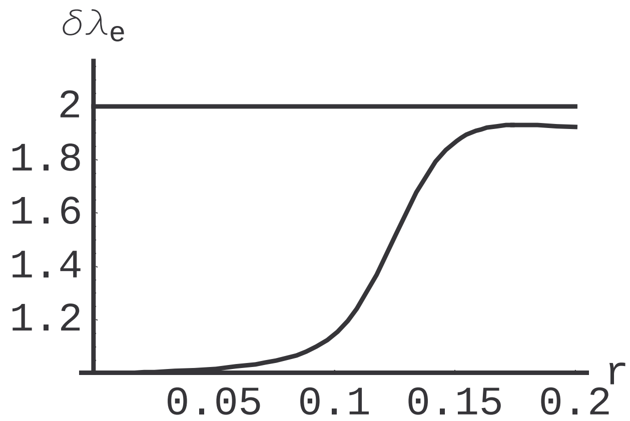
<u>Open problem:</u> To find a simple rule to calculate A⟦k⟧.

Table of the first sequences $p_1\, p_2 \ldots p_M$ of $X_{p_1\, p_2 \ldots\, p_M}$:

2					
22					
33	222				
44	332 233	2222			
55	442 343 244	3322 2332 2233	22222		
66	255 354 453 552	2244 2343 3333 2442 3432 4422	22233 22332 23322 33222	222222	

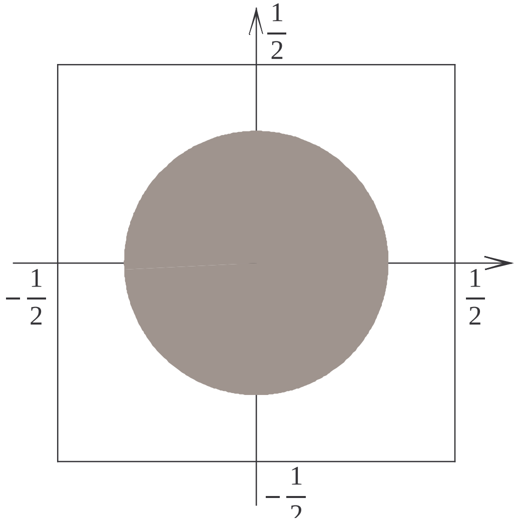


Percolation phenomena. The disks generate a cluster. $\lambda_e^{(1)}$ is computed for 9 disks, $\lambda_e^{(2)}$ correpons to the simular geometry but without the central disk (8 disks)



When r changes from zero to 0.217, the effective conductivity increases for both structures.We have $\lambda_e^{(1)} \approx \lambda_e^{(2)}$ until the point $r = 0.1$. Near the point $r = 0.15$ the effective conductivity of the first material becomes 2 times more despite the fixed relatively small difference of the concentrations (11%).

Regular square array. An exact formula:



$$\lambda_e = 1 + 2\,\rho\text{v} \sum_{m=0}^{\infty} A_m(r^2)\,\rho^m\, r^{2\,m}, \tag{5.1}$$

where

$$A_1(x) = \alpha^{-1}\, 2\,\zeta(\alpha/2),\; A_2(x) = \sum_{n=0}^{\infty} \sigma_{2\,n}^{(2)}\, S_{2\,(n+1)}\, x^{2\,n}, \tag{5.2}$$

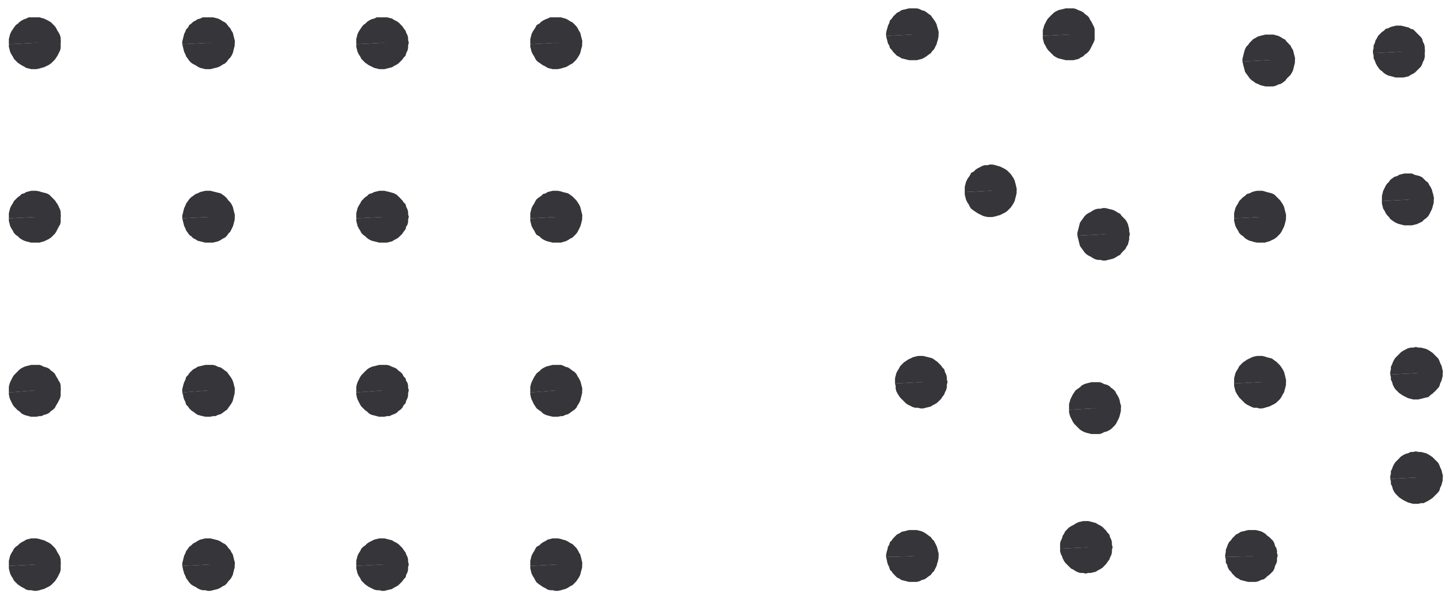
$$A_m(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_{m-1}=0}^{\infty} \sigma_{2\,n_1}^{(2\,n_2+2)}\, \sigma_{2\,n_2}^{(2\,n_3+2)} \dots \sigma_{2\,n_{m-2}}^{(2\,n_{m-1}+2)}\, \sigma_{2\,n_{m-1}}^{(2)}\, S_{2\,(n_1+1)}\, x^{2\,(n_1+n_2 \dots + n_{m-1})},$$

$$\sigma_{2\,l}^{(2\,n)} = C_{2\,l+2\,n-1}^{2\,l}\, S_{2\,(n+l)}.$$

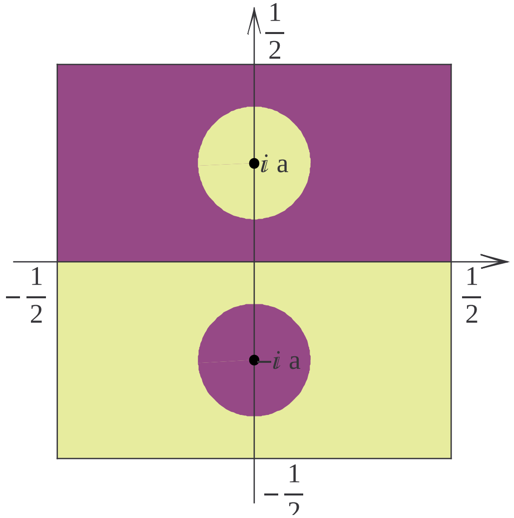
Note. Formulas (5.1)-(5.2) are exact.

An extremal property of the square array:

Consider random arrays (``shaking" geometries) when the fibers are allowed to move randomly inside the periodicity cell according certain uniform distribution. The periodic array of the fibers has lower effective conductivity than any array obtained by the random shaking of the fibers.



Fiber-layer composite:



$$\lambda_e^x = \lambda_0^x\left(1 - 4\,\rho\pi\, r^2 - 4\,\rho^3(2\,\rho + 1)\,\pi\, r^4\, \mathrm{Re}\wp(2\, i\, a)\right),$$

where $\lambda_0^x = \frac{\lambda_1+\lambda_2}{2}$, $\wp(z)$ is the Weierstrass function;

$$\lambda_e^y = \lambda_0^y\left(1 + 4\,\rho\pi\, r^2 + 4\,\rho^3(2\,\rho + 1)\,\pi\, r^4\, \mathrm{Re}\wp(2\, i\, a)\right),\ \text{where } \lambda_0^y = \frac{2}{1/\lambda_1+1/\lambda_2}.$$

6. Pearmeabilty

Equations: $\Delta w = 1$ (Poisson equation) (6.1)

$w(x, y)$ is doubly periodic (6.2)

$w(x, y) = 0$ on ∂D (6.3)

(6.1)-(6.3) is reduced to the following problem for harmonic function $u(z)$:

$\Delta u = 0$ (6.4)

$u(x, y)$ is doubly periodic (6.5)

$$u(x, y) = -\frac{1}{4\pi}\left(S_2 x^2 - (2\pi - S_2) y^2\right) + \frac{1}{2\pi n} \ln|\sigma(z - a_k)| \quad \text{on} \quad \partial D \qquad (6.6)$$

Longitudinal permeability: $K = -\int_D w(x, y)\, d\sigma$

Constructive formula: $K = -\left(\sum_{m=1}^{n} \frac{1}{\ln r_k}\right)^{-1} \left(1 - \sum_{\mathbf{s},j} c_{\mathbf{s},j} \frac{r_1^{2 s_1} r_2^{2 s_2} \dots r_n^{2 s_n}}{\ln^{t_1} r_1 \ \ln^{t_2} r_2 \dots \ln^{t_n} r_n}\right)$, $\mathbf{s} = (s_1, s_2, \dots, s_n)$