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Note: Effective diffusion coefficient in heterogeneous media

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Studies of the transport properties of heterogeneous materials[1–3] have a long history, back to the Maxwell-Garnett (MG) paper dated 1904.[4] Since then, several attempts to generalize the MG effective medium theory have been made. In particular, while the MG theory assumes equal particle concentrations in the matrix and inclusions, a more general theory was developed that allows a concentration jump at the matrix-inclusion boundary.[5] In this Note, we show that the extended effective medium theory[5,6] leads to an exact solution for the effective diffusion coefficient in a periodic layered media. To do this we take advantage of the fact that such a medium can be described by a one-dimensional model.

Consider one-dimensional heterogeneous medium formed by periodically distributed matrix and inclusion regions with the diffusion coefficients D_1 and D_2, respectively, as schematically shown in Fig. 1(a). The effective medium theory[5] replaces the heterogeneous periodic medium by a representative element consisting of a matrix and one inclusion, which are embedded into the effective media with the diffusion coefficient D_{eff} (Fig. 1). The corresponding concentrations are denoted by $c_{eff}(x)$, $c_1(x)$, $c_2(x)$, and $c_3(x)$.

It is assumed that the effective concentration describes a stationary solution of the diffusion equation, $c_{eff}(x) = -gx$, $x < x_1$, $x > x_4$, where g is a constant concentration gradient. In the representative element, $x_1 < x < x_4$ the stationary concentration profile is given by

$$c_1 = \alpha_1 x + \beta_1 (\text{in } I), \quad c_2 = \alpha_2 x + \beta_2 (\text{in } II), \quad c_3 = \alpha_3 x + \beta_3 (\text{in } III), \tag{1}$$

where $x_3 - x_2$ is the length of the inclusion layer, $x_2 - x_1 = x_4 - x_3$ is the half-length of the matrix layer, and $x_4 - x_1 = L$ is the period of the layered medium (Fig. 1(a)). We have chosen the boundary conditions of the form:

$$c_{eff}\Big|_{x=x_1} = \frac{1}{\chi} c_1\Big|_{x=x_1}, \; c_1\Big|_{x=x_2} = \frac{1}{k} c_2\Big|_{x=x_2}, \quad c_2|_{x=x_3} = k c_3|_{x=x_3}, \; c_3|_{x=x_4} = \chi c_{eff}|_{x=x_4}, \tag{2}$$

$$D_{eff}\frac{\partial c_{eff}}{\partial x}\Big|_{x=x_1} = D_1 \frac{\partial c_1}{\partial x}\Big|_{x=x_1}, \; D_1\frac{\partial c_1}{\partial x}\Big|_{x=x_2} = D_2\frac{\partial c_2}{\partial x}\Big|_{x=x_2}, \quad D_2\frac{\partial c_2}{\partial x}\Big|_{x=x_3} = D_1\frac{\partial c_3}{\partial x}\Big|_{x=x_3}, \; D_1\frac{\partial c_3}{\partial x}\Big|_{x=x_4} = D_{eff}\frac{\partial c_{eff}}{\partial x}\Big|_{x=x_4}. \tag{3}$$

In Eq. (2), coefficients k and χ characterize the concentration jumps at the inclusion-matrix and matrix-effective medium boundaries, respectively. A typical diffusion concentration profile is shown in the Fig. 2.

One can find D_{eff} using Eqs. (1)–(3) together with the requirement of the conservation of the total number of the particles,

$$\int_{x_1}^{x_4} c_{eff}(x)dx = \int_{x_1}^{x_2} c_1(x)dx + \int_{x_2}^{x_3} c_2(x)dx + \int_{x_3}^{x_4} c_3(x)dx. \tag{4}$$

The result is

$$D_{eff} = \frac{D_1 D_2}{(1 - f + kf)\left(D_1(1-f) + \frac{D_1}{k} f\right)}, \tag{5}$$

where f is the fraction of the period occupied by the inclusion (Fig. 2):

$$f = \frac{x_3 - x_2}{x_4 - x_1} = \frac{x_3 - x_2}{L}. \tag{6}$$

Taking k equal to unity, we recover the expression for D_{eff} provided by the initial MG theory,[4] which assumes the equal probabilities of finding diffusing particles in the matrix and inclusion,

$$D_{eff} = \frac{D_1 D_2}{D_2(1-f) + D_1 f}. \tag{7}$$

It is interesting that the extended effective medium theory[5] provides an exact solution for the effective diffusion coefficient. To show this, take advantage of the Lifson-Jackson formula,[7] which gives D_{eff} of a particle diffusing in a one-dimensional periodic potential $U(x)$, $U(x) = U(x + L)$, with a periodic diffusion coefficient, $D(x + L) = D(x)$, where

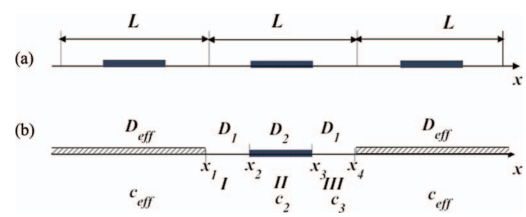

FIG. 1. Periodic heterogeneous medium (a) and its representation by the effective medium theory (b).

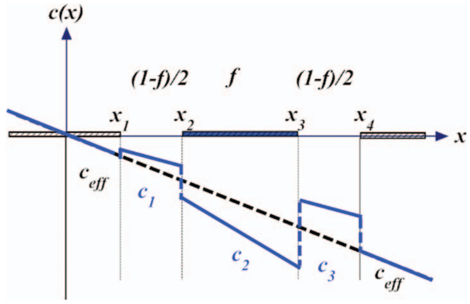

FIG. 2. The concentration profile (solid line) (the dashed line shows $c_{eff}(x) = -gx$ inside the representative element).

L is the period. According to this formula:

$$D_{eff} = \frac{1}{\langle \exp(-\beta U(x)\rangle \langle \exp(\beta U(x)/D(x)\rangle}, \qquad (8)$$

where $\beta = (k_B T)^{-1}$ with k_B is the Boltzmann constant and T is the absolute temperature, and $\langle F(x)\rangle$ is the average of function $F(x)$ over the period L,

$$\langle F(x)\rangle = \frac{1}{L}\int_0^L F(x)dx. \qquad (9)$$

Taking $U(x) = 0$ and $D(x) = D_1$ in the matrix (regions *I* and *III*), and $U(x) = -\beta^{-1}\ln(k)$, $D(x) = D_2$ in inclusion (region *II*) and performing the integration, we find that Eq. (8) leads to the result Eq. (5).

In summary, a closed formula for the effective diffusion coefficient in a heterogeneous medium with periodically distributed inclusions is derived using the extended effective medium theory.[5] It is shown that the expression for the effective diffusion coefficient is an exact result, since it follows from Lifson-Jackson formula.[7]

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