

## Note: Effective diffusion coefficient in heterogeneous media

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Studies of the transport properties of heterogeneous materials<sup>1–3</sup> have a long history, back to the Maxwell-Garnett (MG) paper dated 1904.<sup>4</sup> 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.<sup>5</sup> In this Note, we show that the extended effective medium theory<sup>5,6</sup> 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<sup>5</sup> 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

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

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:

$$\begin{aligned} c_{eff} \Big|_{x=x_1} &= \frac{1}{\chi} c_1 \Big|_{x=x_1}, & c_1 \Big|_{x=x_2} &= \frac{1}{k} c_2 \Big|_{x=x_2}, \\ c_2 \Big|_{x=x_3} &= k c_3 \Big|_{x=x_3}, & c_3 \Big|_{x=x_4} &= \chi c_{eff} \Big|_{x=x_4}, \end{aligned} \quad (2)$$

$$D_{eff} \frac{\partial c_{eff}}{\partial x} \Big|_{x=x_1} = D_1 \frac{\partial c_1}{\partial x} \Big|_{x=x_1}, \quad D_1 \frac{\partial c_1}{\partial x} \Big|_{x=x_2} = D_2 \frac{\partial c_2}{\partial x} \Big|_{x=x_2}, \quad (3)$$

$$D_2 \frac{\partial c_2}{\partial x} \Big|_{x=x_3} = D_1 \frac{\partial c_3}{\partial x} \Big|_{x=x_3}, \quad D_1 \frac{\partial c_3}{\partial x} \Big|_{x=x_4} = D_{eff} \frac{\partial c_{eff}}{\partial x} \Big|_{x=x_4}.$$

In Eq. (2), coefficients  $k$  and  $\chi$  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,

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

The result is

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

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

$$f = \frac{x_3 - x_2}{x_4 - x_1} = \frac{x_3 - x_2}{L}. \quad (6)$$

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

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

It is interesting that the extended effective medium theory<sup>5</sup> provides an exact solution for the effective diffusion coefficient. To show this, take advantage of the Lifson-Jackson formula,<sup>7</sup> 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

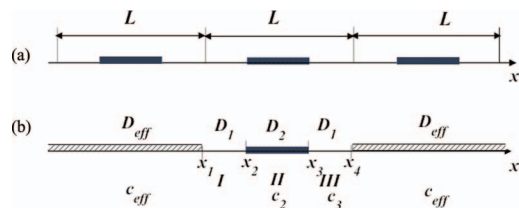


FIG. 1. Periodic heterogeneous medium (a) and its representation by the effective medium theory (b).

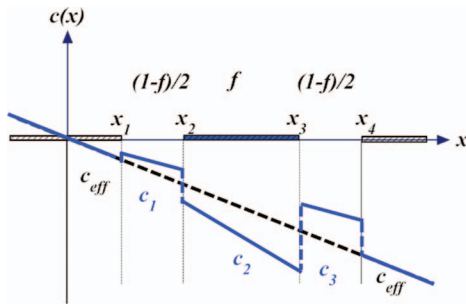


FIG. 2. The concentration profile (solid line) (the dashed line shows  $c_{eff}(x) = -gx$  inside the representative element).

$L$  is the period. According to this formula:

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

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  $L$ ,

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

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.<sup>5</sup> It is shown that the expression for the effective diffusion coefficient is an exact result, since it follows from Lifson-Jackson formula.<sup>7</sup>

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