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Transport in Ordered and Disordered Porous Media IV: Computer Generated Porous Media for Three-Dimensional Systems

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Abstract. In the method of volume averaging, the difference between ordered and disordered porous media appears at two distinct points in the analysis, i.e. in the process of spatial smoothing and in the closure problem. In the *closure problem*, the use of spatially periodic boundary conditions is *consistent with* ordered porous media and the fields under consideration when the length-scale constraint, $r_0 \ll L$ is satisfied. For disordered porous media, spatially periodic boundary conditions are an approximation in need of further study.
In the *process of spatial smoothing*, average quantities must be removed from area and volume integrals in order to extract *local* transport equations from *nonlocal* equations. This leads to a series of geometrical integrals that need to be evaluated. In Part II we indicated that these integrals were constants for ordered porous media provided that the weighting function used in the averaging process contained the *cellular average*. We also indicated that these integrals were constrained by certain order of magnitude estimates for disordered porous media. In this paper we verify these characteristics of the geometrical integrals, and we examine their values for pseudo-periodic and uniformly random systems through the use of computer generated porous media.

Key words:

0. Nomenclature

Roman Letters

$A_{\beta\sigma}$ interfacial area of the β–σ interface associated with the local closure problem, m^2.

$A_{\beta e}$ area of entrances and exits for the β-phase contained within the averaging system, m^2.

a_i $i = 1, 2, 3$ gaussian probability distribution used to locate the position of particles.

$\mathbf{I}$ unit tensor.

L general characteristic length for volume averaged quantities, m.

L_ε characteristic length for ε_β, m.

L_ψ characteristic length for $\langle \psi_\beta \rangle^\beta$, m.

ℓ_σ characteristic length for the σ-phase particles, m.
ℓ_σ^0 reference characteristic length for the σ-phase particles, m.
ℓ_β characteristic length for the β-phase, m.
ℓ_i $i = 1, 2, 3$ lattice vectors, m.
m convolution product weighting function.
$m_\mathcal{V}$ special convolution product weighting function associated with the traditional volume average.
n_i $i = 1, 2, 3$ integers used to locate the position of particles.
$\mathbf{n}_{\beta\sigma}$ unit normal vector pointing from the β-phase toward the σ-phase.
$\mathbf{n}_{\beta e}$ outwardly directed unit normal vector at the entrances and exits of the β-phase.
r_p position vector locating the centroid of a particle, m.
r_σ gaussian probability distribution used to determine the size of a particle, m.
r_0 characteristic length of an averaging region, m.
$\mathbf{r}$ position vector, m.
r_m support of the weighting function m, m.
$\mathcal{V}$ averaging volume, m^3.
V_β volume of the β-phase contained in the averaging volume, $\mathcal{V}$, m^3.
$\mathbf{x}$ positional vector locating the centroid of an averaging volume, m.
$\mathbf{x}_0$ reference position vector associated with the centroid of an averaging volume, m.
$\mathbf{y}$ position vector locating points relative to the centroid, m.
$\mathbf{y}_\beta$ position vector locating points in the β-phase relative to the centroid, m.

Greek Letters

γ_β indicator function for the β-phase.
$\delta_{\beta\sigma}$ Dirac distribution associated with the β–σ interface.
ε_β $V_\beta/\mathcal{V}$, volume average porosity.
ε ℓ/L, small parameter in the method of spatial homogenization.
σ_{a_i} standard deviation of a_i.
σ_r standard deviation of r_σ.
$\langle\psi_\beta\rangle^\beta$ intrinsic phase average of ψ_β.

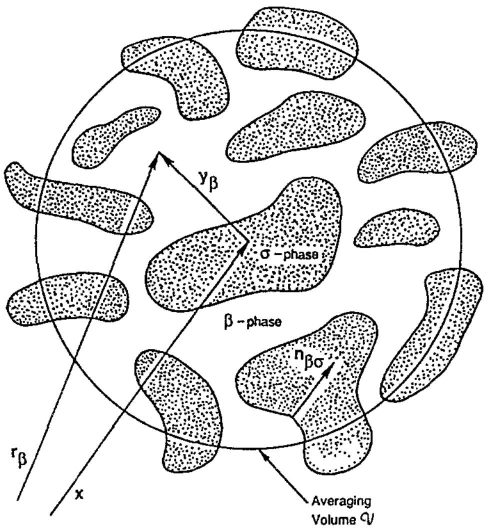

Fig. 1. A two-phase system.

1. Introduction

In the analysis of transport processes taking place in the β–σ system illustrated in Figure 1, the traditional method of volume averaging leads to integrals of averaged quantities of the form

$$\frac{1}{\mathcal{V}}\int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}\langle\psi_\beta\rangle^\beta \,\mathrm{d}A, \qquad \frac{1}{\mathcal{V}}\int_{V_\beta} \langle\psi_\beta\rangle^\beta \,\mathrm{d}V.$$

These integrals are obtained with the weighting function $m_{\mathcal{V}}$ discussed in Sec. 1 of Part II, and if the average quantity, $\langle\psi_\beta\rangle^\beta$, remains inside the integral a nonlocal theory results (Quintard and Whitaker, 1990). In order to remove $\langle\psi_\beta\rangle^\beta$ from these integrals, one can make use of a Taylor series expansion and the geometrical theorems presented in Appendix B of Part II to obtain

$$\begin{aligned}\frac{1}{\mathcal{V}}\int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}\langle\psi_\beta\rangle^\beta \,\mathrm{d}A = {}& -(\nabla\varepsilon_\beta)\langle\psi_\beta\rangle^\beta - \\ & -\nabla\langle\mathbf{y}_\beta\rangle\cdot\nabla\langle\psi_\beta\rangle^\beta - \\ & -\tfrac{1}{2}\nabla\langle\mathbf{y}_\beta\mathbf{y}_\beta\rangle\colon\nabla\nabla\langle\psi_\beta\rangle^\beta - \cdots\cdots\cdots\end{aligned} \tag{1.1}$$

$$\begin{aligned}\frac{1}{\mathcal{V}}\int_{V_\beta} \langle\psi_\beta\rangle^\beta \,\mathrm{d}V = {}& \varepsilon_\beta\langle\psi_\beta\rangle^\beta + \langle\mathbf{y}_\beta\rangle\cdot\nabla\langle\psi_\beta\rangle^\beta + \\ & +\tfrac{1}{2}\langle\mathbf{y}_\beta\mathbf{y}_\beta\rangle\colon\nabla\nabla\langle\psi_\beta\rangle^\beta + \\ & +\cdots\cdots\cdots\end{aligned} \tag{1.2}$$

Here it is understood that $\langle\psi_\beta\rangle^\beta$ is evaluated at the position, $\mathbf{x}+\mathbf{y}_\beta$, when it appears inside either integral, and that it is evaluated at the centroid when it appears outside the integral sign. An example of Equation (1.1) is given by Equation (2.11) in Part II, while Equation (1.2) represents the form illustrated by Equation (2.30) in Part III.

1.1. ORDERED MEDIA

For ordered media one would use the generalized averaging procedure described in Part II to replace Equation (1.1) with

$$m * [\delta_{\beta\sigma}\mathbf{n}_{\beta\sigma}\gamma_\beta\langle\psi_\beta\rangle^\beta_m] = 0 \tag{1.3}$$

provided m contained the cellular average indicated by $m_V * m_V$. The analogous form for Equation (1.2) would be

$$m * \langle\psi_\beta\rangle^\beta_m = m * \gamma_\beta\langle\psi_\beta\rangle^\beta_m + [m * (\gamma_\beta\mathbf{y}\mathbf{y})]\colon \nabla\nabla\langle\psi_\beta\rangle^\beta_m + \cdots\cdots \tag{1.4}$$

and since $m * (\gamma_\beta\mathbf{y}\mathbf{y})$ is on the order of $(m * \gamma_\beta)r_m^2$ the higher order terms can be discarded whenever the following length-scale constraint is satisfied

$$r_m^2 \ll L_\psi^2. \tag{1.5}$$

For a simple spatially periodic porous medium, such as an array of uniform spheres, r_m is on the order of ℓ_β and Equation (1.5) can be related to the work of Levy (1983) and many others by expressing it as

$$\varepsilon^2 \ll 1. \tag{1.6}$$

Here ε is the small parameter (ℓ/L) in the method of spatial homogenization (Bensoussan *et al*; 1978; Sanchez-Palencia, 1980). For ordered systems, we see that the simplification of the integral given by Equation (1.4) depends *only* upon the field of the averaged quantity, i.e. on $\nabla\nabla\langle\psi_\beta\rangle^\beta_m$. For disordered systems we need to be concerned both with the field of the average quantity and the geometrical integrals. Large gradients in either of these quantities will prohibit the development of a local theory. Since the geometrical integrals associated with ordered porous media can be evaluated exactly for any given model, our studies in Parts IV and V will be entirely restricted to the traditional volume average as suggested by Equations (1.1) and (1.2).

1.2. DISORDERED MEDIA

For disordered and nonhomogeneous porous media the first terms on the right hand side of both Equation (1.1) and Equation (1.2) are always part of the development of a local theory, while the third terms always remain as an error. Turning our attention to Equation (1.1), which takes the trivial form of Equation (1.3) for ordered media, we can estimate $\nabla\langle\mathbf{y}_\beta\mathbf{y}_\beta\rangle$ as

$$\nabla\langle\mathbf{y}_\beta\mathbf{y}_\beta\rangle = \mathbf{O}(\varepsilon_\beta r_0^2/L_\varepsilon) \tag{1.7}$$

Since the third term in Equation (1.1) is always discarded relative to $\varepsilon_\beta\nabla\langle\psi_\beta\rangle^\beta$ (see Equation (2.14), Part II), we see that the restriction

$$\nabla\langle\mathbf{y}_\beta\mathbf{y}_\beta\rangle\colon \nabla\nabla\langle\psi_\beta\rangle^\beta \ll \varepsilon_\beta\nabla\langle\psi_\beta\rangle^\beta \tag{1.8}$$

produces the constraint

$$r_0^2 \ll L_\varepsilon L_\psi. \tag{1.9}$$

The third term on the right-hand side of Equation (1.2) is always neglected relative to $\langle\psi_\beta\rangle^\beta$ and this leads to the analogous form of Equation (1.5) given by

$$r_0^2 \ll L_\psi^2. \tag{1.10}$$

The inequalities given by Equations (1.5), (1.9), and (1.10) would appear to impose severe constraints on local theories in the neighborhood of a boundary. However, the detailed studies of Prat (1989, 1990, 1991, 1992) concerning the volume averaged heat conduction equation near a boundary suggest that these constraints are overly severe.

At this point it should be clear that the second terms on the right hand side of Equations (1.1) and (1.2) play a key role in the simplification of the integrals for disordered media. Thus our primary concern in this paper is the behavior of $\langle\mathbf{y}_\beta\rangle$ and $\nabla\langle\mathbf{y}_\beta\rangle$ for disordered media since these geometrical quantities control the importance of $\nabla\langle\psi_\beta\rangle^\beta$ in the representations given by Equations (1.1) and (1.2). Here we should recall our definition of a disordered porous medium given by

> A porous medium is disordered *with respect to* an
> averaging volume $\mathcal{V}$ when $\nabla\langle\mathbf{y}_\beta\rangle \ll \mathsf{I}$.

This says nothing about the magnitude of $\langle\mathbf{y}_\beta\rangle$ which appears in Equation (1.2); however, one can construct the estimate

$$\langle\mathbf{y}_\beta\rangle\,|_{\mathbf{r}_2} = \langle\mathbf{y}_\beta\rangle\,|_{\mathbf{r}_1} + \mathbf{0}[(\mathbf{r}_2 - \mathbf{r}_1)\cdot\nabla\langle\mathbf{y}_\beta\rangle] \tag{1.11}$$

to conclude that

$$\langle\mathbf{y}_\beta\rangle = \mathbf{0}(L\nabla\langle\mathbf{y}_\beta\rangle^\beta) \tag{1.12}$$

provided a point $\mathbf{r}_1$ exists at which $\langle\mathbf{y}_\beta\rangle$ is zero or on the order of $L\nabla\langle\mathbf{y}_\beta\rangle$. This result leads to

$$\langle\mathbf{y}_\beta\rangle\cdot\nabla\langle\psi_\beta\rangle^\beta \ll \langle\psi_\beta\rangle^\beta \tag{1.13}$$

whenever $\nabla\langle \mathbf{y}_\beta \rangle$ is small compared to one, thus we will tend to focus our attention on $\nabla\langle \mathbf{y}_\beta \rangle$ in our study of ordered and disordered systems.

The characterization of the microstructure of a two-phase system is a well-developed field of research, and it is appropriated for us to clarify our specific objectives. The geometrical quantities involving averages of $\mathbf{y}_\beta$ play an important role in the theory of volume averaging, and we are interested in the behavior of these quantities for a variety of systems that are encountered in practical applications or used for theoretical analysis. Periodic systems play an important role in the theory of spatial homogenization (Bensoussan *et al.* 1978; Sanchez–Palencia, 1980), generalized Taylor dispersion theory (Brenner, 1980), and they are used extensively in numerical studies at the particle-scale level (Zick and Homsy, 1982). Natural systems, on the other hand, are usually thought of as disordered or uncorrelated. A traditional description of disordered systems is provided by the Boolean schemes discussed by Matheron (1967) or by the system of randomly distributed spheres described by Salacuse and Stell (1982), Torquato (1984, 1986), and Rubinstein and Torquato (1989). Several statistical properties associated with the geometry of these microstructures can be derived (Strieder and Aris, 1963), in addition to bounds for transport coefficients such as the effective diffusivity and the permeability (Weissberg, 1963; Prager, 1969). Our objectives in this study are completely different, i.e. we are interested in the mathematical behavior of $\langle \mathbf{y}_\beta \rangle$, $\nabla\langle \mathbf{y}_\beta \rangle$, $\langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle$, etc. for a given realization of a two-phase system. In order to accurately calculate these quantities, we have generated two and three-dimensional systems of cubic particles for systems which we refer to as periodic, pseudo-periodic, and uniformly random. In all cases the *orientation* of the particles is uniform and parallel to the lattice vectors that describe a unit cell.

2. Computer Generated Two-Phase Systems

In this section we describe the different types of two-phase systems that are used to calculate the geometrical parameters that appear in the method of volume averaging. In order to perform calculations in a very accurate and efficient manner, we restrict our numerical studies to systems of cubic or square particles as illustrated in Figure 2.

2.1. PERIODIC SYSTEMS

The generation of a periodic system is achieved by locating the centroid of the pth particle according to

$$\mathbf{r}_p = n_1\ell_1 + n_2\ell_2 + n_3\ell_3. \tag{2.1}$$

Here n_1, n_2, and n_3 are integers, ℓ_1, ℓ_2, and ℓ_3 are the lattice vectors, and the description of the system is complete when the size of the cube (represented by the edge length ℓ_σ) is specified. The averaging volume is taken to be a *representative volume* and is therefore a cube.

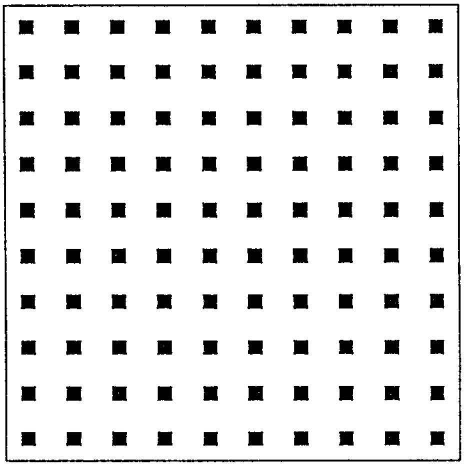

Fig. 2. Periodic system of cubes parameters: $\ell_1 = \ell_2 = \ell_\beta,\ \varepsilon_\beta = 0.91$.

2.2. PSEUDO-PERIODIC SYSTEMS

Pseudo-periodic systems are *defined* in this study by a perturbation of Equation (2.1). The position of a particle is obtained by a random process identified as

$$\mathbf{r}_p = (n_1 + a_1)\ell_1 + (n_2 + a_2)\ell_2 + (n_3 + a_3)\ell_3 \tag{2.2}$$

in which a_1, a_2, and a_3 have a gaussian probability distribution with a mean value of zero. In addition, the characteristic length of a particle, ℓ_σ, is given by

$$\ell_\sigma = \ell_\sigma^0 + r_\sigma, \quad \ell_\sigma \geqslant 0 \tag{2.3}$$

in which ℓ_σ^0 is a constant and r_σ is a random function having a gaussian probability distribution and a mean value of zero. The standard deviations for a_i and r_σ are denoted by σ_{a_i} and σ_r. It should be clear that all values of $\mathbf{r}_p$ and ℓ_σ cannot be chosen at random since this would lead to overlapping particles. Some rule is needed to deal with this problem, and we have chosen to reduce the value of ℓ_σ when it is necessary to avoid overlapping. Examples of pseudo-periodic systems are illustrated in Figures 3, 4, and 5.

2.3. UNIFORMLY RANDOM SYSTEMS

In these systems the position, $\mathbf{r}_p$, is determined by a uniformly random spatial distribution, while the length of a particle is determined by Equation (2.3). A particle having a position $\mathbf{r}_p$ and length ℓ_σ is retained in the array if it does not overlap with all previously generated particles. If it does overlap it is discarded as opposed to reducing the value of ℓ_σ in order to eliminate overlap as was done with pseudo-periodic systems. Our method of generating uniformly random systems is similar in nature to the PCS models studied by Torquato (1986). An example of a

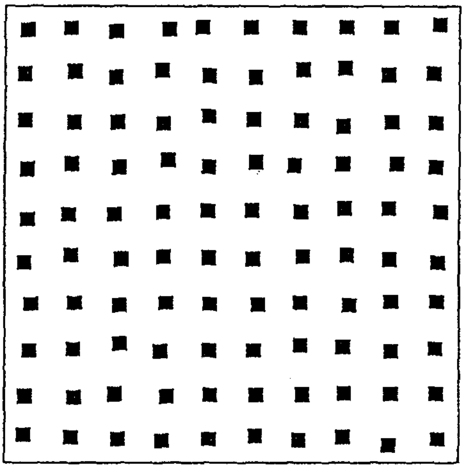

Fig. 3. Pseudo-periodic system I. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$; $\sigma_{a_1} = \sigma_{a_2} = \sigma_{a_3} = 0.05$; $\ell_\sigma^0 = 0.3\ell_\beta$, $\varepsilon_\beta = 0.91$.

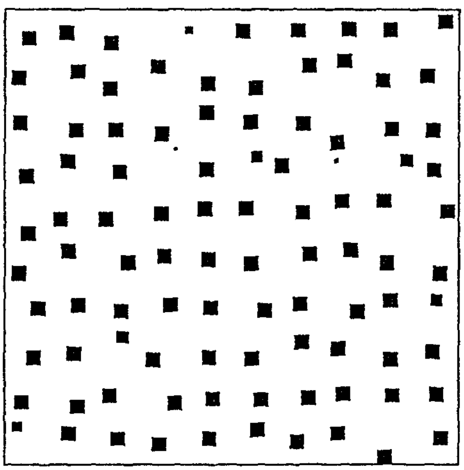

Fig. 4. Pseudo-periodic system II. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$; $\sigma_{a_1} = \sigma_{a_2} = \sigma_{a_3} = 0.15$; $\ell_\sigma^0 = 0.3\ell_\beta$, $\varepsilon_\beta = 0.91$.

uniformly random system is illustrated in Figure 6, and it would appear that this system is quite similar to the one shown in Figure 5. The geometrical parameters for these systems are presented in the next section and they indicate that appearances can be deceiving.

3. Three-Dimensional Geometrical Properties

In this section we present results for $\mathbf{i}\cdot\nabla\langle \mathbf{y}_\beta\rangle\cdot\mathbf{i}$ for periodic, pseudo-periodic, and uniformly random systems. A two-dimensional representation of the computational network is shown in Figure 7, and for *periodic systems* ℓ_σ and ℓ_β are related by

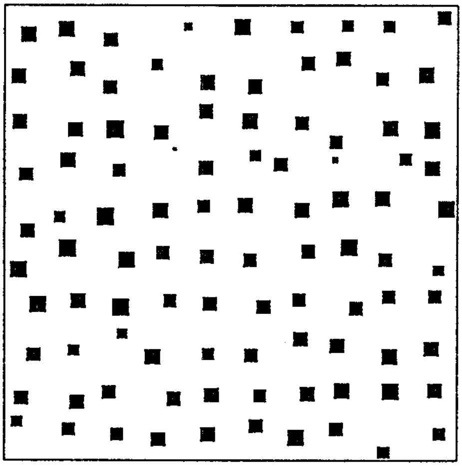

Fig. 5. Pseudo-periodic system III. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$, $\sigma_{a_1} = \sigma_{a_2} = \sigma_{a_3} = 0.15$; $\ell_\sigma^0 = 0.3\ell_\beta$, $\varepsilon_\beta = 0.912$.

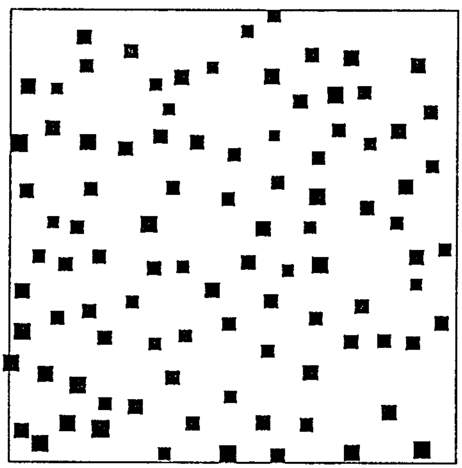

Fig. 6. Uniformly random system. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$, $\sigma_r = 0.10\ell_\sigma^0$, $\varepsilon_\beta = 0.914$.

$$\frac{\ell_\sigma}{\ell_\beta} = (1 - \varepsilon_\beta^0)^{1/3}. \tag{3.1}$$

One begins the calculation by choosing a value of ε_β^0 so that ℓ_σ/ℓ_β is specified and the periodic array can be constructed. The calculation for *pseudo-periodic systems* is more complex. One chooses a value of ℓ_σ^0/ℓ_β according to

$$\frac{\ell_\sigma^0}{\ell_\beta} = (1 - \varepsilon_\beta^0)^{1/3} \tag{3.2}$$

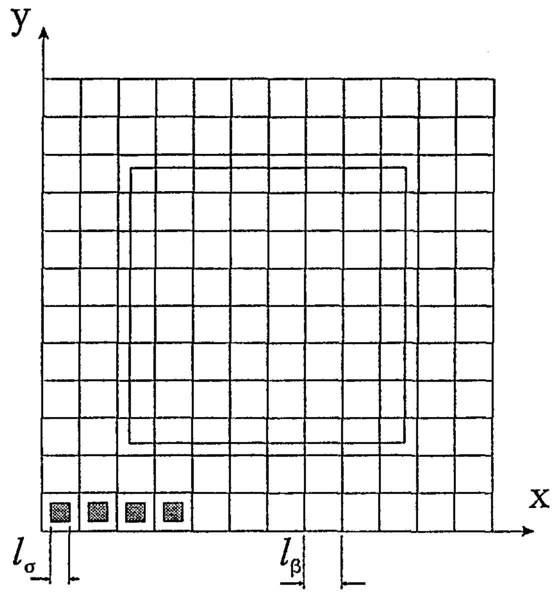

Fig. 7. Computational network.

in which ε_β^0 is taken to be the same value as that used in Equation (3.1). Starting with an empty network, the position and size of a particle are chosen by Equations (2.2) and (2.3) with the lattice vectors given by

$$\ell_1 = \mathbf{i}\ell_\beta, \qquad \ell_2 = \mathbf{j}\ell_\beta, \qquad \ell_3 = \mathbf{k}\ell_\beta. \tag{3.3}$$

According to Equation (2.2), the particle associated with the cell located by $n_1\ell_1 + n_2\ell_2 + n_3\ell_3$ need not be located in that cell. The calculation using Equations (2.2) and (2.3) is repeated so that a particle is associated with every cell in the network. When an overlap occurs, the particle size is diminished until the overlap disappears. This method of eliminating the overlap skews the particle-size distribution that is originally controlled by the gaussian distribution of $\mathbf{r}_\sigma$. The particle-size distribution is weighted in favor of the smaller particles, thus the calculated porosity for pseudo-periodic systems is always larger than ε_β^0. Skewing of the particle size distribution could be diminished by discarding particles that overlap and repeating the calculation indicated by Equations (2.2) and (2.3); however, this was considered to be unnecessary for the construction of pseudo-periodic systems when moderate values of σ_a and σ_r were used.

For *uniformly random systems*, the value of ℓ_σ^0/ℓ_β is determined by Equation (3.2). The first particle is located in the computational network in a random manner and its size is determined by Equation (2.3). The size and position of all subsequent particles are chosen in the same manner; however, when overlap occurs the particle is discarded. This procedure also skews the particle-size distribution in favor of the smaller particles since they more easily fit into the computational network, and this leads to values of the porosity larger than ε_β^0. By trial and error, one could adjust the choice of ε_β^0 in Equation (3.2) in order to produce a porosity identical to that used in the periodic systems; however, the computational costs associated with this procedure do not appear to be justified.

In order to determine $\nabla\langle \mathbf{y}_\beta\rangle$ we wish to avoid calculating $\langle \mathbf{y}_\beta\rangle$ as a function of position in order to evaluate the gradient. With the aid of one of the geometrical theorems presented in Part II we can represent $\nabla\langle \mathbf{y}_\beta\rangle$ in terms of an area integral over $A_{\beta e}$, the area of entrances and exits of the β-phase contained within the averaging volume, $\mathcal{V}$. The following special form can be extracted from Equation (2.12b) of Part II

$$\frac{1}{\mathcal{V}}\int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}\mathbf{y}_\beta \,\mathrm{d}A = -\nabla\langle \mathbf{y}_\beta\rangle \tag{3.4}$$

while the divergence theorem can be used to provide

$$\frac{1}{\mathcal{V}}\int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}\mathbf{y}_\beta \,\mathrm{d}A + \frac{1}{\mathcal{V}}\int_{A_{\beta e}} \mathbf{n}_{\beta e}\mathbf{y}_\beta \,\mathrm{d}A = \varepsilon_\beta \mathsf{I}. \tag{3.5}$$

These two results lead to the very convenient computational form given by

$$\nabla\langle \mathbf{y}_\beta\rangle = -\varepsilon_\beta \mathsf{I} + \frac{1}{\mathcal{V}}\int_{A_{\beta e}} \mathbf{n}_{\beta e}\mathbf{y}_\beta \,\mathrm{d}A. \tag{3.6}$$

With this result, the calculation of $\nabla\langle \mathbf{y}_\beta\rangle$ for cubic particles and cubic averaging volumes is very straightforward when all cubes are oriented parallel to the coordinate system. Even so, the computation becomes time consuming when thousands of particles are contained in an averaging volume.

3.1. PERIODIC SYSTEMS

In the case of periodic systems, $\nabla\langle \mathbf{y}_\beta\rangle$ can be calculated analytically for simple systems, and this is done in Appendix A for an array of uniform spheres and in Appendix B for an array of uniform cubes. These studies lead to

$$\nabla\langle \mathbf{y}_\beta\rangle = \mathbf{0}[(1-\varepsilon_\beta)]. \tag{3.7}$$

The value of $\mathbf{i}\cdot\nabla\langle \mathbf{y}_\beta\rangle\cdot\mathbf{i}$ for a periodic system is illustrated in Figure 8 and there we see that $\nabla\langle \mathbf{y}_\beta\rangle$ is not differentiable at certain points. This occurs when the surface of the averaging volume coincides with the surface of the particles and this characteristic has been discussed by Veverka (1981), Howes and Whitaker (1985), and Mlš (1987). It should be clear that the cellular average of $\nabla\langle \mathbf{y}_\beta\rangle$ is zero and that $\nabla\langle \mathbf{y}_\beta\rangle$ is independent of the size of the averaging volume when the averaging volume is composed of unit cells.

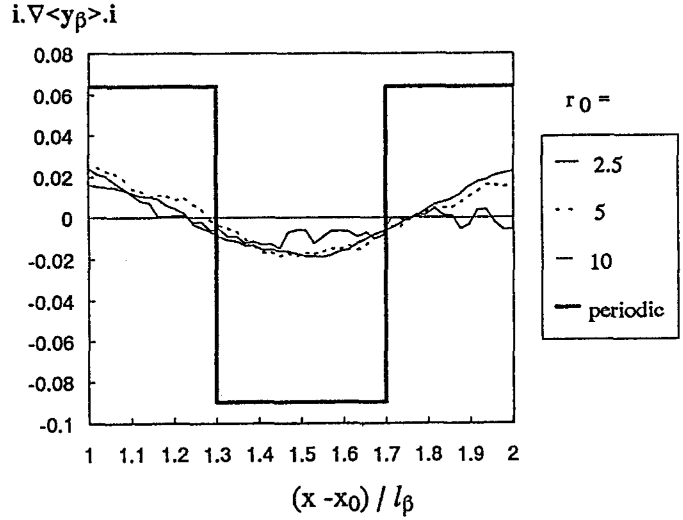

Fig. 8. Spatial variation of $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for periodic and pseudo-periodic systems. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$, $\sigma_{a_1} = \sigma_{a_2} = \sigma_{a_3} = 0.15$, $\ell_\sigma^0 = 0.6\ell_\beta$, $\varepsilon_\beta \sim 0.64$.

3.2. PSEUDO-PERIODIC SYSTEMS

The behavior of $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for a pseudo-periodic system is also illustrated in Figure 8 for three different averaging volumes, all of which are cubes made of unit cells. The pseudo-periodic system under consideration is the one illustrated in Figure 5. While this system has much the same *appearance* as the uniformly random system shown in Figure 6, the periodic nature is clearly evident in Figure 8. The values of $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ exhibit spatial variations on a length scale smaller than ℓ_β; however, when the size of the averaging volume is $20\ell_\beta \times 20\ell_\beta \times 20\ell_\beta$ the small scale variations are negligible. The results shown in Figure 8 clearly indicate that variations on the order of the length-scale ℓ_β are not influenced by the size of the averaging volume, thus the pseudo-periodic system shown in Figure 5 contains a *fingerprint* of the periodic system from which it was derived. Clearly a cellular average should be used to analyze transport processes in a pseudo-periodic system having the characteristics illustrated in Figure 5.

3.3. DISORDERED SYSTEMS

The spatial variations of $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for uniformly random systems are represented in Figure 9 along with the curve for a periodic system. For a single averaging volume having the size $24\ell_\beta \times 24\ell_\beta \times 24\ell_\beta$, the uniformly random system qualifies as a disordered porous medium in terms of our definition. Smaller averaging volumes would obviously contain small-scale fluctuations as indicated in Figure 8 for the case $\mathcal{V} = 5\ell_\beta \times 5\ell_\beta \times 5\ell_\beta (r_0/\ell_\beta = 2.5)$; however, the results in Figure 9 clearly demonstrate that $\nabla \langle \mathbf{y}_\beta \rangle \ll \mathsf{I}$ when the averaging volume is sufficiently large.

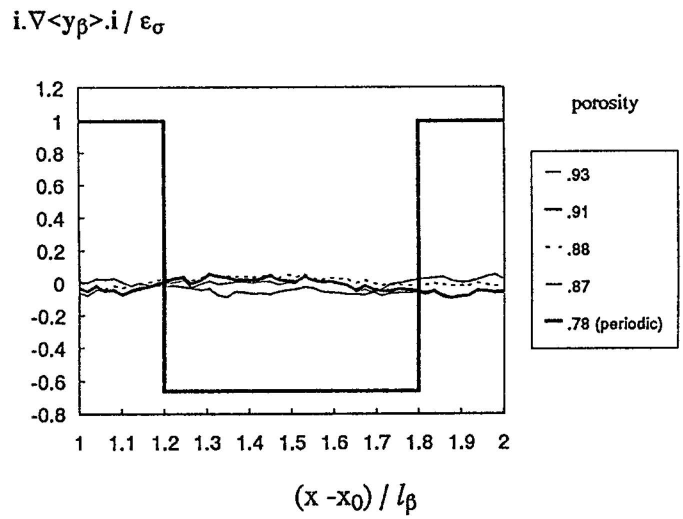

Fig. 9. Spatial variations of $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for uniformly random systems. Parameters: $\ell_1 = \ell_2 = \ell_3 = \ell_\beta$, $\ell_\sigma^0 = 0.6\ell_\beta$, $\sigma_r = 0.10\ell_\sigma^0$, $r_0 = 12\ell_\beta$.

The four uniformly random systems illustrated in Figure 9 all have relatively high porosities. This results from the excessive computer time required to place particles in the system after 10% of the space has been filled. Generation of uniformly random systems with porosities in the neighborhood of $\varepsilon_\beta \sim 0.4$ would appear to be computationally impossible at this time, and perhaps not necessary since real porous media are not formed in this manner. For packed beds of particles, the computer simulation employed by Chu and Ng (1989) contains many attractive features; however, their approach becomes computationally impossible for a Gaussian distribution of particle sizes and their results are restricted to spheres of almost the same size.

Our results for three-dimensional systems are quite limited; however, they clearly establish that $\nabla \langle \mathbf{y}_\beta \rangle$ is a key indicator of *order* and *disorder* and that knowledge of this parameter can be used to make decisions concerning the simplification of the integrals in Equations (1.1) and (1.2). In our studies presented in this section we have used averaging volumes that are unit cells, i.e. cubic averaging volumes are used with cubic systems. One could say that these unit cells are *representative elementary volumes*; however, this terminology does not conform exactly with Bear's (1972, page 19) definition of an REV. It is of some interest to explore these same problems using an averaging volume that *is not representative* in order to see what effect the configuration of $\mathcal{V}$ has upon the geometrical parameters. To achieve this, we have used a circular averaging area and two-dimensional arrays of squares, and these results are described in the Part V.

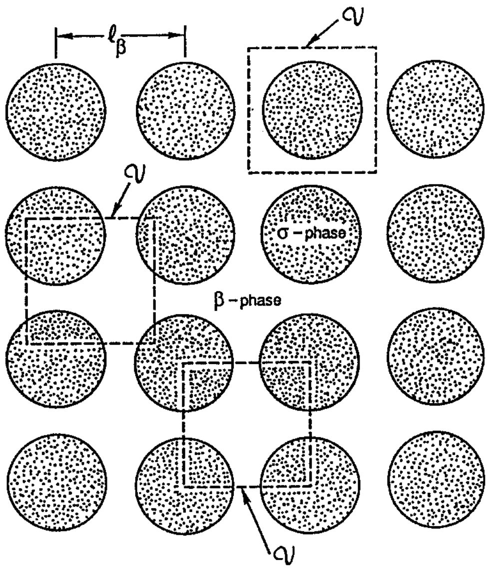

Fig. A-1. Three-dimensional array of spheres.

4. Conclusions

In this paper we have evaluated $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ and $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for ordered arrays of spheres and cubes in order to verify our comments made in Parts I and II concerning these geometrical quantities. In addition, we have evaluated $\mathbf{i} \cdot \nabla \langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ for computer generated pseudo-periodic and uniformly random two-phase systems. The results, while limited in scope, suggest that our definition of disordered media is consistent with systems generated by some random process.

Appendix A: Geometrical Parameters for Regular Arrays of Spheres

In this appendix we consider some of the geometrical characteristics of the three-dimensional regular array of spheres illustrated in Figure A-1. The diameter of the spheres is $2a$ and the center-to-center distance between the spheres in the x-direction is taken to be the characteristic length, ℓ_β. In Figure A-2 we have illustrated an averaging volume having a centroid at $x = -1/2(\ell_\beta - 2a)$, and with the averaging volume we can develop the following expressions for $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$.

$$\text{I.} \quad 0 \leqslant x \leqslant \frac{\ell_\beta}{2} - a, \tag{A.1a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)x, \tag{A.1b}$$

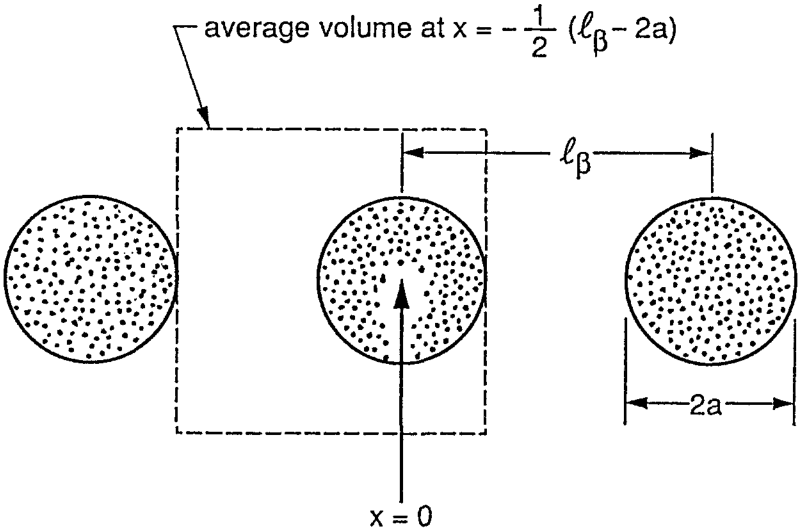

Fig. A-2. One-dimensional displacement of the averaging volume.

$$\text{II.}\quad \frac{\ell_\beta}{2} - a \leqslant x \leqslant \frac{\ell_\beta}{2} + a, \tag{A.2a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)(x - \tfrac{1}{4}[\zeta^2(3 - \zeta)\ell_\beta]), \tag{A.2b}$$

$$\zeta = \frac{1}{a}\left\{x - \left(\frac{\ell_\beta}{2} - a\right)\right\}, \tag{A.2c}$$

$$\text{III.}\quad \frac{\ell_\beta}{2} + a < x \leqslant \ell_\beta, \tag{A.3a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)(x - \ell_\beta). \tag{A.3b}$$

Values of $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ are deduced by periodicity for values of x outside $[0, \ell_\beta]$. These results are plotted in Figure A-3 and from that figure and/or Equations (A.1) and (A.2) we have the following estimates

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \mathbf{0}((1 - \varepsilon_\beta)\ell_\beta), \tag{A.4}$$

$$\frac{\partial}{\partial x}(\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}) = \mathbf{0}((1 - \varepsilon_\beta)) \tag{A.5}$$

which were given in Part I as Equation (1.14).

The first order geometrical parameter is the crucial parameter in the averaging process. To illustrate the order of magnitude analysis for higher order geometrical parameters, we give below the algebraic expression for only one component of the second intrinsic geometrical parameter, namely $\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i}$

$$\text{I.}\quad 0 \leqslant x \leqslant \frac{\ell_\beta}{2} - a, \tag{A.6a}$$

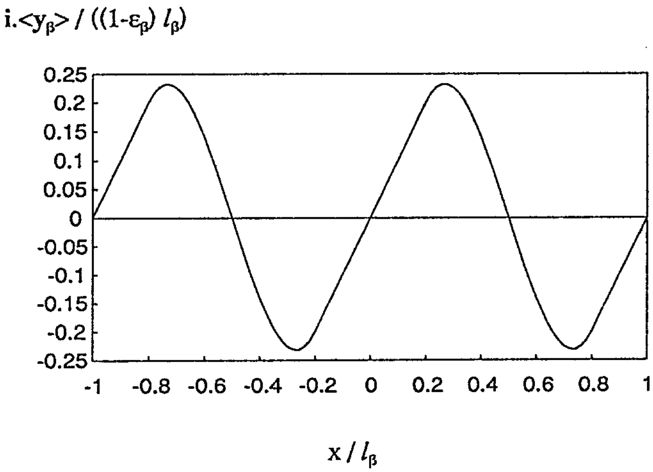

Fig. A-3. Values of $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ as a function of x (Arrays of Spheres $a/\ell_\beta = 0.3$).

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} + \pi (f(-x+a) - f(-x+a)) \right) \tag{A.6b}$$

where

$$f(u) = u^3 \left(\frac{u^2}{5} + \frac{u}{2} x + \frac{x^2 - a^2}{3} \right),$$

II. $\dfrac{\ell_\beta}{2} - a \leqslant x \leqslant \dfrac{\ell_\beta}{2} + a,$ (A.7a)

$$\begin{aligned} \mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = {} & \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} + \pi \left(f(-x+a) - f\left(-\frac{\ell_\beta}{2}\right) \right. \right. \\ & \left. \left. + \, g\left(\frac{\ell_\beta}{2}\right) - g(-\ell_\beta - x - a) \right) \right) \end{aligned} \tag{A.7b}$$

where

$$g(u) = u^3 \left(\frac{u^2}{5} + \frac{u}{2}(x - \ell_\beta) + \frac{(x-\ell_\beta)^2 - a^2}{3} \right),$$

III. $\dfrac{\ell_\beta}{2} + a \leqslant x \leqslant \ell_\beta,$ (A.8a)

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} + \pi (g(\ell_\beta - x + a) - g(\ell_\beta - x - a)) \right). \tag{A.8b}$$

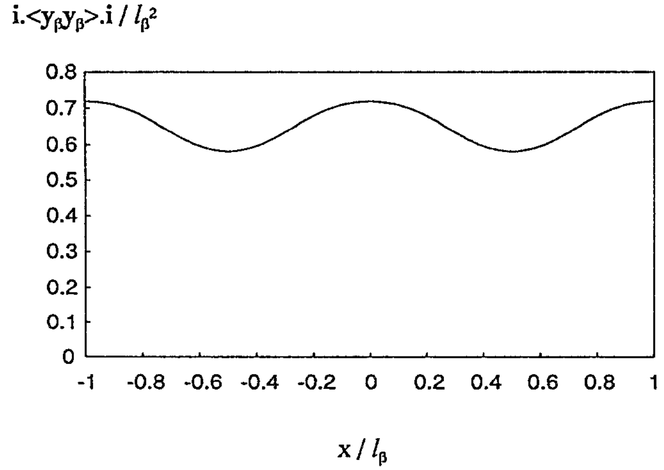

Fig. A-4. Values of $\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ as a function of x (Arrays of Spheres, $a/\ell_\beta = 0.3$).

These results are plotted in Figure A-4. Such expressions suggest the following estimate

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = 0(\ell_\beta^2). \tag{A.9}$$

However, one should keep in mind that ℓ_β also plays the role of r_0 in this calculation, and for larger averaging volumes we would obtain the estimates listed in Section 1 of this paper which are confirmed in Part V.

Appendix B: Geometrical Parameters for Regular Arrays of Cubes

In this appendix we consider some of the geometrical characteristics of the three-dimensional regular array of *cubes*. The notation is similar to that used in Appendix A, $2a$ being the length of the cube edges. We obtain the following expressions for $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$.

I. $$0 \leqslant x \leqslant \frac{\ell_\beta}{2} - a, \tag{B.1a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)x, \tag{B.1b}$$

II. $$\frac{\ell_\beta}{2} - a \leqslant x \leqslant \frac{\ell_\beta}{2} + a, \tag{B.2a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)\left(x - \frac{\ell_\beta}{2a}\left[x - \frac{\ell_\beta}{2} + a\right]\right), \tag{B.2b}$$

III. $$\frac{\ell_\beta}{2} + a \leqslant x \leqslant \ell_\beta, \tag{B.3a}$$

$$\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i} = (1 - \varepsilon_\beta)(x - \ell_\beta). \tag{B.3b}$$

Values of $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ are deduced by periodicity for values of x outside $[0,\ \ell_\beta]$. These results are plotted in Figure B-1.

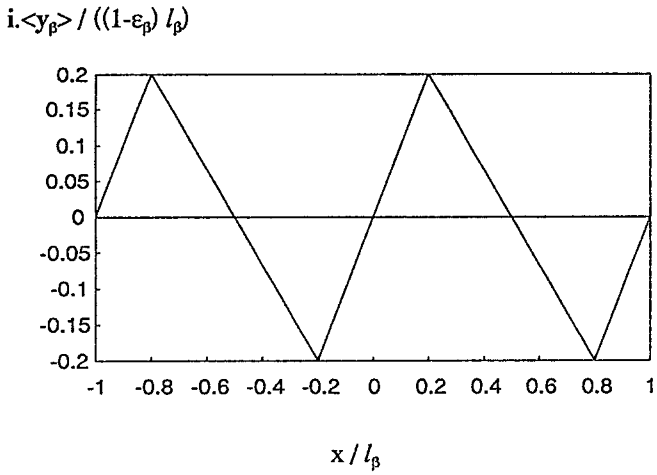

Fig. B-1. Values of $\langle \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ as a function of x (Arrays of Cubes $a/\ell_\beta = 0.3$).

For the component $\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ of the second intrinsic geometrical parameter, we have

$$\text{I.} \quad 0 \leqslant x \leqslant \frac{\ell_\beta}{2} - a, \tag{B.4a}$$

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} - \frac{8}{3} a^3 (a^2 + 3x^2) \right), \tag{B.4b}$$

$$\text{II.} \quad \frac{\ell_\beta}{2} - a \leqslant x \leqslant \frac{\ell_\beta}{2} + a, \tag{B.5a}$$

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} - \frac{4}{3} a^2 \left((a - x)^3 + \right.\right.$$

$$\left.\left. + \frac{\ell_\beta^3}{4} - (\ell_\beta - a - x)^3 \right) \right), \tag{B.5b}$$

$$\text{III.} \quad \frac{\ell_\beta}{2} + a \leqslant x \leqslant \ell_\beta, \tag{B.6a}$$

$$\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i} = \frac{1}{\ell_\beta^3} \left(\frac{\ell_\beta^5}{12} - \frac{4}{3} a^2 ((\ell_\beta + a - x)^3 - \right.$$

$$\left. - (\ell_\beta - a - x)^3) \right). \tag{B.6b}$$

These results are plotted in Figure B-2, and they suggest the same estimates as those discussed in Appendix A.

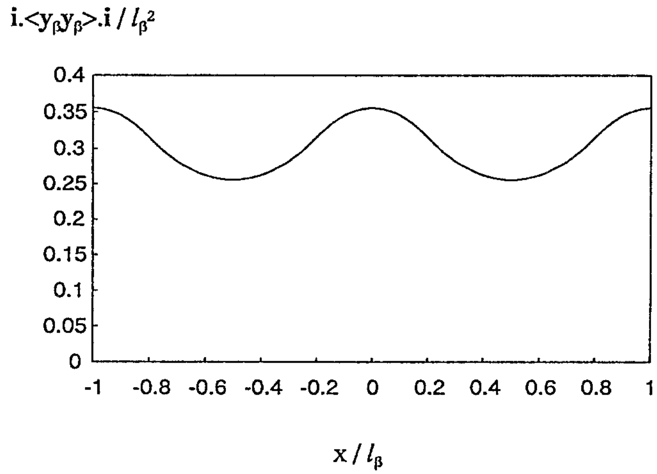

Fig. B-2. Values of $\mathbf{i} \cdot \langle \mathbf{y}_\beta \mathbf{y}_\beta \rangle \cdot \mathbf{i}$ as a function of x (Arrays of Cubes, $a/\ell_\beta = 0.3$).

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