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SLOW FLOW THROUGH A PERIODIC ARRAY OF SPHERES

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Abstract—Slow flow through a periodic array of spheres is studied theoretically, and the drag force by the fluid on a sphere forming the periodic array is calculated using a modification of the method developed by Hashimoto (1959). Results for the complete range of volume fraction c of spheres are given for simple cubic, body-centered cubic, and face-centered cubic arrays and these agree well with the corresponding values reported by previous investigators. Also, series expansions for the drag force to $0(c^{10})$ are derived for each of these cubic arrays. The method is also applied to determine the drag force to $0(c^3)$ on infinitely long cylinders in square and hexagonal arrays.

1. INTRODUCTION

Slow flows of incompressible Newtonian fluids through an array of fixed particles occur in many physical processes and therefore their study is important from both the practical and the theoretical point of view. We consider an idealized case in which the particles are equal-sized spheres of radius a^* arranged in periodic arrays and assume that the Reynolds number of the flow is much smaller than unity so that the fluid motion satisfies the well known Stokes equations of motion. Our primary goal here is to calculate the drag force F exerted by the fluid moving with average speed U on a representative sphere in the assembly as a function of the volume fraction c of the spheres. In addition, though, the method of solution to be developed yields expressions for the local velocity and the pressure fields.

Hasimoto (1959) was probably the first to successfully treat the case of dilute arrays ($c \ll 1$). He derived the periodic fundamental solution to the Stokes equations of motion and, after expanding the velocity profile in terms of this fundamental solution and its derivatives, obtained an expression for F for the three cubic arrays (simple, body-centered and face-centered). For the simple cubic array he found that

$$K^{-1} = 1 - 1.7601\, c^{1/3} + c - 1.5593\, c^2 + 0(c^{8/3}), \qquad [1]$$

$$\text{where } K = \frac{F}{6\pi\mu U a^*}, \qquad [2]$$

and μ is the viscosity of the fluid. Clearly, [1] is meaningless for c beyond approximately 0.2 when K becomes negative. Hasimoto's results for body-centered and face-centered arrays are also quantitatively similar to [1]. Although in principle, it should have been possible to calculate additional terms in [1] using Hasimoto's method, this does not appear to have been done to date.

In this paper, we modify Hasimoto's treatment and calculate K over the complete range of c for all three of the cubic arrays. We find first of all that the expression for the velocity given by Hasimoto is incomplete and that the extra terms affect the coefficients of [1] to $0(c^{10/3})$ and beyond. On using the complete representation for the velocity we then derive an expression for K to $0(c^{10})$ which appears to converge for $0 < c/c_{max} < 0.85$, where c_{max} is the maximum concentration of spheres for a given packing and equals $\pi/6$, $\sqrt{3}\pi/8$, and $\sqrt{2}\pi/6$, respectively for a simple cubic, a body-centered cubic and a face-centered cubic array. For $0.85 < c/c_{max} < 1$ the drag is obtained, as explained in section 3, by a "direct substitution" evaluation of the linear equations relating the coefficients of the formal solution.

Recently, Zick & Homsy (1982) also computed the drag on a sphere in the above three cubic arrays. Using Hasimoto's (1959) fundamental solution, they obtained a set of integral equations for the unknown stress vector at the surface of a sphere which they then solved numerically. Our results are in good agreement with theirs—as well as with Sorensen & Stewart's (1974) value for touching spheres in a simple cubic array.

We also consider the slow flow through periodic arrays of infinitely long circular cylinders. For the square array Hasimoto (1959) obtained

$$\frac{F'}{4\pi\mu U}=\frac{1}{-\frac{1}{2}\ln c-0.738+c+0(c^2)} \tag{3}$$

where F' is the magnitude of the drag force exerted by the fluid per unit length of a cylinder. We have extended Hasimoto's method and have calculated $F'/4\mu U$ to $0(c^3)$ for square and hexagonal arrays. For $c<0.25$ the series give results which are in excellent agreement with those obtained by the present authors (Sangani & Acrivos 1982a) using a numerical method which is similar to Galerkin's method.

The procedure to be described here for solving the creeping flow equations in periodic arrays can also be easily extended and applied to the problem of calculating the effective elastic moduli of composite materials which consists of cubic arrangements of spherical particles embedded in an isotropic matrix with different elastic properties. The analogous case of determining the effective thermal conductivity in periodic array of spheres has also been treated in detail by the present authors (Sangani & Acrivos 1982b).

2. THE FORMAL SOLUTION FOR THE SLOW FLOW IN A CUBIC ARRAY OF SPHERES

2.1 *Governing equations*

Let us consider the steady motion of a viscous fluid through an array of spheres whose centers are located at

$$\mathbf{r_n}=h(n_1\mathbf{a}_{(1)}+n_2\mathbf{a}_{(2)}+n_3\mathbf{a}_{(3)})\quad (n_1,n_2,n_3=0,\pm 1,\pm 2,\ldots), \tag{4}$$

where $\mathbf{a}_{(1)}$, $\mathbf{a}_{(2)}$ and $\mathbf{a}_{(3)}$ are the basic vectors determining the unit cell of the array and their components for the three cubic arrays are listed in appendix 1. Since our analysis is restricted to cubic arrays, we assume, without loss of generality, that the mean flow is along the x_1-axis. As mentioned in the introduction, we take the Reynolds number of the flow to be very small so that the fluid velocity satisfies the Stokes equations of motion and the continuity equation

$$\mu\Delta u_i=\frac{\partial p}{\partial x_i}\quad\left(\Delta=\frac{\partial^2}{\partial x_1{}^2}+\frac{\partial^2}{\partial x_2{}^2}+\frac{\partial^2}{\partial x_3{}^2}\right), \tag*{[5]}$$

$$\frac{\partial u_i}{\partial x_i}=0, \tag*{[6]}$$

where p is the pressure and u_i is the velocity of the fluid at the point (x_1, x_2, x_3). Because of the periodicity and the symmetry of the system, our solution must satisfy the conditions (Sorensen & Stewart 1974)

$$u_1(x_1,x_2,x_3)=u_1(x_1,-x_2,x_3)=u_1(x_1,x_2,-x_3)=u_1(-x_1,x_2,x_3) \tag*{[7]}$$

$$u_2(x_1,x_2,x_3)=-u_2(x_1,-x_2,x_3)=u_2(x_1,x_2,-x_3)=-u_2(-x_1,x_2,x_3) \tag*{[8]}$$

$$u_3(x_1,x_2,x_3)=u_3(x_1,-x_2,x_3)=-u_3(x_1,x_2,-x_3)=-u_3(-x_1,x_2,x_3) \tag*{[9]}$$

$$u_2(x_1, x_2, x_3) = u_3(x_1, x_3, x_2) \quad [10]$$

$$u_1(x_1, x_2, x_3) = u_1(x_1, x_3, x_2) \quad [11]$$

$$\mathbf{u}(\mathbf{r} + \mathbf{r_n}) = \mathbf{u}(\mathbf{r}) \quad [12]$$

$$\mathbf{u} = 0 \quad \text{on sphere,} \quad [13]$$

where [13] refers to the no-slip boundary condition at the surface of the spheres and u_1, u_2 and u_3 are the components of the velocity along the x_1, x_2 and x_3 axes, respectively. As mentioned in the introduction, we shall follow Hasimoto's treatment in order to solve [5]–[6] subject to the conditions [7]–[13]. Before starting our calculation we non-dimensionalize the distances with h, the components of velocity with U and the pressure with $\mu U/h$.

2.2 *The formal solution*

A periodic fundamental solution (v_i, q) to the creeping flow equations can be obtained by solving

$$\Delta v_i = \frac{\partial q}{\partial x_i} + \delta_{i1} \sum_{\mathbf{n}} \delta(\mathbf{r} - \mathbf{r_n}), \quad (14)$$

$$\frac{\partial v_i}{\partial x_i} = 0, \quad (15)$$

where $\delta(\mathbf{r} - \mathbf{r_n})$ is Dirac's delta function defined

$$\int_\tau \delta(\mathbf{r} - \mathbf{r_n})\, d\mathbf{r} = \begin{cases} 1 & \text{when } \mathbf{r_n} \in \tau \\ 0 & \text{when } \mathbf{r_n} \notin \tau \end{cases} \quad (16)$$

and

$$\delta(\mathbf{r} - \mathbf{r_n}) = 0 \text{ for } \mathbf{r} \neq \mathbf{r_n}. \quad (17)$$

As shown by Hasimoto (1959)

$$v_i = v_0 \delta_{i1} - \frac{1}{4\pi}\left(S_1 \delta_{i1} - \frac{\partial^2 S_2}{\partial x_1 \partial x_i}\right) \quad (18)$$

$$\frac{\partial q}{\partial x_i} = -\frac{\delta_{i1}}{\tau_0} + \frac{\partial^2 S_1}{\partial x_1 \partial x_i}, \quad (19)$$

where τ_0 is the non-dimensional volume of the unit cell which equals the triple scalar product of the basic vectors, i.e.

$$\tau_0 = \mathbf{a}_{(1)} \cdot [\mathbf{a}_{(2)} \times \mathbf{a}_{(3)}]. \quad [20]$$

Also, S_1 and S_2 in the above equations are given by

$$S_1 = \frac{1}{\pi \tau_0} \sum_{\mathbf{k_n} \neq 0} \frac{e^{-2\pi i(\mathbf{k_n} \cdot \mathbf{r})}}{k_n^2}, \quad S_2 = \frac{-1}{4\pi^3 \tau_0} \sum_{\mathbf{k_n} \neq 0} \frac{e^{-2\pi i(\mathbf{k_n} \cdot \mathbf{r})}}{k_n^4} \quad [21]$$

where

$$\mathbf{k_n} = n_1 \mathbf{b}_{(1)} + n_2 \mathbf{b}_{(2)} + n_3 \mathbf{b}_{(3)} \quad [22]$$

are vectors in the reciprocal lattice given by

$$\mathbf{k_n} \cdot \mathbf{a}_{(i)} = n_i \quad (i = 1, 2, 3). \qquad [23]$$

The reciprocal lattice vectors $b_{(i)}$ $(i = 1, 2, 3)$ for simple, body-centered, and face-centered cubic arrays are given in appendix 1. Further, as shown by Hasimoto, S_1 and S_2 are solutions of

$$\Delta S_2 = S_1 \qquad [24]$$

and

$$\Delta S_1 = 4\pi \left[\frac{1}{\tau_0} - \sum_{\mathbf{n}} \delta(\mathbf{r} - \mathbf{r_n})\right]. \qquad [25]$$

It is important to note that the derivatives of S_1 are harmonic functions and therefore automatically satisfy the homogeneous part of [5]. To obtain a completely general solution to u_i, we add to the fundamental solution v_i, the derivatives of v_i and S_1 multiplied by some unknown coefficients. From this sum we omit those terms which do not meet any of the conditions [5]–[11] listed in Section 2.1, and thus arrive at the following expressions for the components of the velocity and for the pressure:

$$u_1 = U_0 - \frac{1}{4\pi}\left\{\mathbf{G}\left(S_1 - \frac{\partial^2 S_2}{\partial x_1^2}\right) + \mathbf{H}\frac{\partial^2 S_1}{\partial x_1^2} - \mathbf{L}\left(\frac{\partial^4}{\partial x_2^4} - 6\frac{\partial^4}{\partial x_2^2 \partial x_3^2} + \frac{\partial^4}{\partial x_3^4}\right) S_1\right\} \qquad [26]$$

$$u_2 = \frac{1}{4\pi}\left\{\mathbf{G}\frac{\partial^2 S_2}{\partial x_1 \partial x_2} - \mathbf{H}\frac{\partial^2 S_1}{\partial x_1 \partial x_2} - \mathbf{L}\frac{\partial}{\partial x_1}\left(\frac{\partial^3}{\partial x_2^3} - 3\frac{\partial^3}{\partial x_3^2 \partial x_2}\right) S_1\right\} \qquad [27]$$

$$u_3 = \frac{1}{4\pi}\left\{\mathbf{G}\frac{\partial^2 S_2}{\partial x_1 \partial x_3} - \mathbf{H}\frac{\partial^2 S_1}{\partial x_1 \partial x_3} - \mathbf{L}\frac{\partial}{\partial x_1}\left(\frac{\partial^3}{\partial x_3^3} - 3\frac{\partial^3}{\partial x_2^2 \partial x_3}\right) S_1\right\} \qquad [28]$$

$$\frac{\partial p}{\partial x_i} = -\frac{6\pi a K}{\tau_0}\delta_{i1} + \frac{1}{4\pi}\mathbf{G}\frac{\partial^2 S_1}{\partial x_1 \partial x_i} \quad \left(a = \frac{a^*}{h}\right), \qquad [29]$$

where **G**, **H** and **L** are the differential operators

$$\begin{Bmatrix}\mathbf{G}\\ \mathbf{H}\\ \mathbf{L}\end{Bmatrix} = \sum_{M=0}^{\infty} \sum_{m=0}^{m \le 1/2M} \begin{Bmatrix}A_{nm}\\ B_{nm}\\ C_{nm}\end{Bmatrix} \left\{\frac{\partial^{2n}}{\partial x_1^{2n}}\left[\left(\frac{\partial}{\partial \xi}\right)^{4m} + \left(\frac{\partial}{\partial \eta}\right)^{4m}\right]\right\} \quad (M = n + 2m) \qquad [30]$$

with

$$\xi = x_2 + ix_3, \quad \eta = x_2 - ix_3, \qquad [31]$$

and where the unknown coefficients A_{nm}, B_{nm}, and C_{nm} are to be determined by applying the no-slip boundary condition [13] at the surface of the spheres. The above expressions for the components of the velocity differ from those given by Hasimoto (1959) in two important aspects. First, the terms containing the differential operator **L** are absent in Hasimoto's solution. As we shall see presently, if these terms are omitted, the number of equations exceed the number of unknowns. Second, the differential operators defined by [30] are a special form of those given by Hasimoto. As discussed by the present authors (1982b) in their calculation of the effective thermal conductivity of composite materials, [30] is the most convenient representation of these differential operators when dealing with problems involving cubic arrays of spheres.

Since it has been shown by Hasimoto (1959) that

$$A_{00} = 3\pi a K, \quad U_0 = 1 + \frac{2\,B_{00}}{\tau_0}, \tag{32}$$

the evaluation of A_{00} directly yields K.

We now proceed to determine the constants A_{nm}, B_{nm} and C_{nm}.

3. AN EXPRESSION FOR K^{-1} TO $0(c^{10/3})$

In this section we shall illustrate the procedure used by Hasimoto (1959) to determine the unknown constants in [30] and simultaneously obtain an expression for K^{-1} to $0(c^{10/3})$.

Since the solution for the velocity components given by [26]–[28] is periodic, the no-slip boundary condition on the surface of each sphere is satisfied automatically if it is satisfied on surface of a sphere with its center at the origin. Accordingly, we concentrate on the unit cell containing the origin and make use of the expansions of S_1 and S_2 in spherical harmonics near $r = 0$ given by Hasimoto (1959).

$$S_1 = \frac{1}{r} - \bar{c} + \frac{2\pi}{3\tau_0} r^2 + \sum_{n=2}^{\infty} \sum_{m=0}^{m \le n/2} a_{nm}\, Y_{2n}^{4m}(x_1, x_2, x_3) \tag{33}$$

$$S_2 = \frac{r}{2} - \bar{c}_2 - \frac{\bar{c}}{6} r^2 + \frac{\pi r^4}{30\tau_0} + \sum_{n=2}^{\infty} \sum_{m=0}^{m \le n/2} (b_{nm} + \tilde{a}_{nm} r^2) Y_{2n}^{4m}(x_1, x_2, x_3), \tag{34}$$

where

$$Y_n{}^m(x_1, x_2, x_3) = r^n p_n{}^m (\cos\theta) \cos m\phi, \tag{35}$$

with

$$x_1 = r\cos\theta,\; x_2 = r\sin\theta\cos\phi,\; x_3 = r\sin\theta\sin\phi, \tag{36}$$

and $\bar{c}$, $\bar{c}_2$, a_{nm}, b_{nm} and $\tilde{a}_{nm}$ are constants characteristic of the array. Not all of them are independent. Thus as shown by Hasimoto (1959)

$$\tilde{a}_{nm} = \frac{1}{2(4n+3)} \tag{37}$$

and as shown by Zuzowski (1976),

$$\frac{a_{20}}{a_{21}} = \frac{b_{20}}{b_{21}} = 168; \quad \frac{a_{30}}{a_{31}} = \frac{b_{30}}{b_{31}} = -360. \tag{38}$$

The constants $\bar{c}$, a_{nm} and b_{nm} for the three cubic arrays are evaluated in appendix 1.

Substituting [30], [33] and [34] into [26]–[28] and using the equations of appendix 2, [A.23]–[A.33], we obtain expressions for the components of the velocity in terms of Legendre polynomials. By equating to zero the coefficients for $r = a$ of P_0, P_2, P_4 and P_4^4 in u_1 and $P_2^1\, e^{i\phi}$, $P_4^1\, e^{i\phi}$ and $P_4^3\, e^{-3i\phi}$ in $u_2 + iu_3$ we arrive at

$$\frac{4}{3a}\left[1 - \bar{c}a + \frac{2\pi}{3\tau_0} a^3\right] A_{00} - \frac{16\pi}{3\tau_0} B_{00} + \left[\frac{16\pi}{15\tau_0} - 48 b_{20} - 8 a_{20} a^2\right] A_{10}$$

$$+ 48\, a_{20} B_{10} - 48\left[\frac{4}{11}\, a_{20} + 30\, b_{30} + 0(a^2)\right] A_{20} + \frac{8!}{16}\left[\frac{10}{11}\, a_{21} - 90 b_{31}\right.$$

$$\left. + 0(a^2)\right] A_{01} - 8!\, a_{21} C_{00} + 0(a^{12}) = 4\pi \tag{39}$$

$$\left[\frac{2}{3a}-\left(\frac{16\pi}{45\tau_0}+24b_{20}\right)a^2-\frac{132}{77}a_{20}a^4\right]A_{00}+4\left[\frac{1}{a^3}+6a_{20}a^2\right]B_{00}$$

$$+\left[\frac{4}{7a^3}-\left(\frac{13}{11}a_{20}+6!b_{30}\right)a^2+0(a^4)\right]A_{10}+0(a^{10})=0 \quad [40]$$

$$a^4\left[\frac{76}{77}a_{20}-60b_{30}+0(a^2)\right]A_{00}+\left[\frac{24}{7a^3}+0(a^4)\right]A_{10}+\left[\frac{48}{a^5}+0(a^4)\right]B_{10}+0(a^7)=0 \quad [41]$$

$$a^4\left[\frac{20}{11}a_{21}-180\,b_{31}+0(a^2)\right]A_{00}+\left[\frac{10}{88a^5}+0(a^4)\right]A_{01}-\left[\frac{2}{a^5}+0(a^4)\right]C_{00}+0(a^7)=0 \quad [42]$$

$$\left[\frac{1}{3a}-8\left(\frac{\pi}{45\tau_0}-b_{20}\right)a^2+\frac{4}{7}a_{20}a^4\right]A_{00}+2\left[\frac{1}{a^3}-8a^2a_{20}\right]B_{00}$$

$$-\left[\frac{6}{7a^3}-\left(\frac{64}{11}a_{20}+240\,b_{30}\right)a^2+0(a^4)\right]A_{10}+0(a^{10})=0 \quad [43]$$

$$a^4\left[12b_{30}-\frac{1}{77}a_{20}+0(a^2)\right]A_{00}+\left[\frac{6}{7a^3}+0(a^4)\right]A_{10}-\left[\frac{120}{11a^5}+0(a^4)\right]A_{20}$$

$$+\left[\frac{12}{a^5}+0(a^4)\right]B_{10}+0(a^7)=0 \quad [44]$$

$$-8a^4\left[\frac{a_{21}}{11}+90\,b_{31}+0(a^2)\right]A_{00}-\left[\frac{1}{22a^5}+0(a^4)\right]A_{01}+\left[\frac{2}{a^5}+0(a^4)\right]C_{00}$$

$$+0(a^7)=0. \quad [45]$$

Comparing the leading order terms in these equations (when $a \ll 1$) we see that, at most,

$$A_{nm}\sim 0(a^{4M+2}),\ B_{nm}\sim 0(a^{4M+4}),\ C_{nm}\sim 0(a^{4M+8}),$$

$$A_{00}\sim 0(a),\ B_{00}\sim 0(a^3). \quad [46]$$

Solving [39]–[45] for A_{00}, we obtain

$$K^{-1}=1-\bar{c}a+\frac{4\pi a^3}{3\tau_0}-\left(\frac{16\pi^2}{45\tau_0^2}+630\,b_{20}^2\right)a^6-300\,a_{20}b_{20}a^8$$

$$-\left(\frac{262}{7}a_{20}^2+27180\,b_{30}^2\right)a^{10}+0(a^{11}), \quad [47]$$

which agrees to $0(a^6)$ with Hasimoto's (1959) corresponding expression. The above series for K^{-1} can also be recast in terms of the volume fraction of the spheres

$$c=\frac{4\pi a^3}{3\tau_0}. \quad [48]$$

For a simple cubic array, [47] reduces to

$$K^{-1}=1-1.7601\,c^{1/3}+c-1.5593\,c^2+3.9799\,c^{8/3}-3.0734\,c^{10/3}$$

$$+0(c^{11/3}), \quad [49]$$

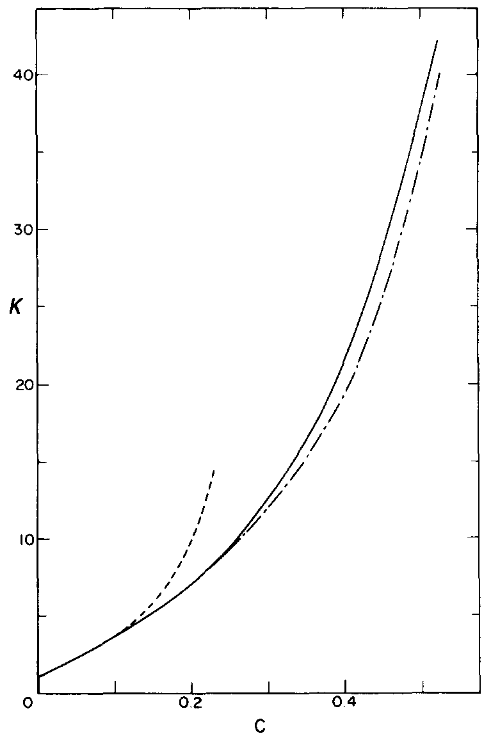

Figure 1. The non-dimensional drag K as a function of the volume fraction c for simple cubic arrays [—exact results, ---[2], —·—[49]].

which, as can be seen in figure 1, is an improvement over Hasimoto's result [1]. The solid curve in that figure represents the numerical results to be discussed in the next section. It should be noted though that the good agreement between [49] and the exact results in figure 1, is only coincidental and that many more terms would be needed to establish the radius of convergence of the above series for K^{-1}.

The process just described for generating the higher order terms in K^{-1} can be continued indefinitely, at least in principle. In the above example, the coefficients of those terms in u_1 and $u_2 + iu_3$ which are multiplied by Legendre polynomials of degree 4 or less were equated to zero, but it can be shown that if the no-slip boundary condition is satisfied by including all Legendre polynomials of degree $4N + 2$ or less, then $3(N + 1)^2$ equations ($N^2 + 3N + 2$ in u_1 and $2N^2 + 3N + 1$ in $u_2 + iu_3$) result. Further, on account of (46), K^{-1} can be determined to $0(a^{8N+7})$ and only $3(N + 1)^2$ number of unknowns [$A_{nm}:(N+2)(N+1)$, $B_{nm}:(N+1)^2$, $C_{nm}:N(N+1)$] can contribute up to this order of approximation in K^{-1}. Thus the number of unknowns equals the number of equations. In Hasimoto's expressions for the velocity, the unknowns C_{nm} were absent and thus the number of unknowns were $N(N+1)$ short of the number of equations. However, since Hasimoto considered terms only up to $N = 0$ his results are unaffected.

In order to proceed with our calculations, we first arrange all the unknown coefficients in a vector **U**, i.e.

$$\mathbf{U} \equiv \Big[\underbrace{A_{00}, A_{10}, A_{20}, A_{01}, \cdots\cdots, A_{1N},}_{N^2+3N+2}\ \underbrace{B_{00}, B_{10}, B_{20}, \cdots\cdots, B_{0N}}_{(N+1)^2}$$

$$\underbrace{C_{00}, C_{10}, \cdots\cdots, C_{1,N-1}}_{N^2+N}\Big]. \qquad [50]$$

Next, we see from [39]–[45] that the equations that result by equating to zero the coefficients of P_0^0, $P_2^0, \cdots P_{4N+2}^{4N}$ in u_1 (which correspond below to the equations given by $i = 1, 2, \cdots,$

N^2+3N+2) and $P_2^{\,1}$, $P_4^{\,1}$, $e^{i\phi}, \cdots P_{4N+2}^{4N+1} e^{i(4N+1)\phi}$ in u_2+iu_3 (equations given below by $i = N^2 + 3N+3, \cdots 3(N+1)^2$) can be represented by

$$\sum_{j=1}^{3(N+1)^2} \{(T^1_{ij} + T^2_{ij} a^2) + (T^3_{ij} + T^4_{ij} a^2)\, a^{2p(i)+1}\}\, U_j = 4\pi a \delta_{i1}, \qquad [51]$$

where the first few coefficients of the matrices $\underline{T}^1$, $\underline{T}^2$, $\underline{T}^3$ and $\underline{T}^4$ were already calculated in [39–[45]. Thus

$$T^1_{1j} = \frac{2}{3}\delta_{j1}, \quad T^1_{21} = 0. \quad T^1_{22} = \frac{4}{7}, \cdots \qquad [52]$$

$$T^2_{1j} = 0, \quad T^2_{2j} = \frac{2}{3}\delta_{j1}, \quad T^2_{3j} = \frac{24}{7}, \cdots \qquad [53]$$

$$T^3_{11} = -\frac{2\bar{c}}{3}, \quad T^3_{12} = \frac{16\pi}{15\tau_0} - 48\, b_{20}, \cdots \qquad [54]$$

$$T^4_{11} = \frac{4\pi}{9\tau_0}, \quad T^4_{12} = -176\tilde{a}_{20}, \quad T^4_{21} = -\frac{132}{7}\tilde{a}_{20}, \cdots \qquad [55]$$

Also $p(i)$ in [51] is the degree of the Legendre polynomial whose coefficient when equated to zero led to the ith equation. Thus,

$$p(1) = 0, p(2) = 2, p(N^2+3N+3) = 2, p(3N^2+6N+3) = 4N+2, \text{etc.} \qquad [56]$$

A computer program can therefore be written to calculate $p(i)$ and the coefficients of the above matrices.

As discussed by the present authors (1982b), the equations resulting from applying the boundary conditions at the surface of a sphere can be solved in either of two ways. The first is a method of successive approximations which generates a series expansion in powers of a—the series method. The second involves determining the constants (A_{nm}, B_{nm}, and C_{nm} in the present case) by matrix inversion for a given value of a—the direct substitution method. We describe here both methods.

In the series method, we expand the constants in power series of a, i.e. we let

$$U_j = \sum_{k=1}^{8N+7} U_j^k a^k. \qquad [57]$$

Substituting [57] into [51] yields the following recursion formula

$$U_l^k = \sum_{i=1}^{S}\sum_{j=1}^{S} T_{li}^{-1}\{4\pi\delta_{i1}\delta_{k1} - T^2_{ij}U_j^{k-2} - T^3_{ij}U_j^{k-2p(i)-1}$$

$$- T^4_{ij}\, U_j^{k-2p(i)-3}\} \qquad (S = 3(N+1)^2), \qquad [58]$$

where $U_l^k = 0$ for $k \leq 0$ and $\underline{T}^{-1}$ is an inverse of $\underline{T}^1$, i.e.

$$\sum_{i=1}^{S} T_{li}^{-1} T^1_{ij} = \delta_{lj}. \qquad [59]$$

Since all the quantities on the r.h.s. of [58] are known or have been previously calculated, series expansions for all the unknowns can be readily obtained from [58]. In particular, since $A_{00} = 3\pi a K$, the series for A_{00} directly gives the asymptotic expansion for K.

In the case of the direct substitution method, [51] are solved directly for selected values of a. Note that in this method even the terms higher than $0(a^{8N+7})$ are retained in these equations.

4. RESULTS

Simple cubic arrays

Listed in table 1 are the coefficients in the series expansion

$$K = \sum_{s=0}^{30} q_s \chi^s, \qquad [60]$$

where

$$\chi = (c/c_{max})^{1/3} \qquad [61]$$

with c_{max}, the volume fraction of the spheres in the touching configuration, equal to $\pi/6 = 0.5236$ for the simple cubic array. We see that the above series fails to give an accurate result for K when χ is close to unity. Indeed, for $\chi = 1$, K increases monotonically to about 39 as the terms in the series [60] are added successively after which it oscillates between 33 and 56. We have tried several of the standard techniques (Van Dyke 1964) for improving the rate of convergence of this series but without success.

On the other hand, the calculation of K via the direct substitution method converged very rapidly as seen in table 2 where values of K for various N and χ are given. The converged values of K as a function of χ are listed in table 3 where they are compared with those from the series solution [60]. We see that they are in agreement to within 1% for $\chi < 0.95$.

As mentioned in the introduction, Zick & Homsy (1982) also calculated K for all the three cubic arrays over the complete range of c. Our results from the direct substitution method are in agreement with theirs to within 0.5%. Our results are similarly in agreement with Sorensen & Stewart's (1974) who found K 42.6 for $\chi = 1$ using a three-dimensional set of stream

Table 1. The coefficients q_s in [60]

S	SC	BCC	FCC
0	0.1000000D+01	0.1000000D+01	0.1000000D+01
1	0.1418649D+01	0.1575834D+01	0.1620994D+01
2	0.2012564D+01	0.2483254D+01	0.2627620D+01
3	0.2331523D+01	0.3233022D+01	0.3518875D+01
4	0.2564809D+01	0.4022864D+01	0.4503759D+01
5	0.2594787D+01	0.4650320D+01	0.5354862D+01
6	0.2873609D+01	0.5281412D+01	0.6240194D+01
7	0.3340163D+01	0.5826374D+01	0.7048893D+01
8	0.3536763D+01	0.6258376D+01	0.7778734D+01
9	0.3504092D+01	0.6544504D+01	0.8380856D+01
10	0.3253622D+01	0.6878396D+01	0.9093106D+01
11	0.2689757D+01	0.7190839D+01	0.1004412D+02
12	0.2037769D+01	0.7268068D+01	0.1099079D+02
13	0.1809341D+01	0.7304025D+01	0.1176754D+02
14	0.1877347D+01	0.7301217D+01	0.1234515D+02
15	0.1534685D+01	0.7236410D+01	0.1261369D+02
16	0.9034708D+00	0.7298014D+01	0.1271545D+02
17	0.2857896D+00	0.7369849D+01	0.1295785D+02
18	−0.5512626D+00	0.7109497D+01	0.1297464D+02
19	−0.1278724D+01	0.6228418D+01	0.1259288D+02
20	0.1013350D+01	0.5235796D+01	0.1233984D+02
21	0.5492491D+01	0.4476874D+01	0.1258161D+02
22	0.4615388D+01	0.3541982D+01	0.1310988D+02
23	−0.5736023D+00	0.2939353D+01	0.1251041D+02
24	−0.2865924D+01	0.3935484D+01	0.1089836D+02
25	−0.4709215D+01	0.5179097D+01	0.1059025D+02
26	−0.6870076D+01	0.3959872D+01	0.1210762D+02
27	0.1455304D+00	0.2297627D+01	0.1221455D+02
28	0.1251891D+02	0.3393390D+01	0.9163566D+01
29	0.9742811D+01	0.4491369D+01	0.5120200D+01
30	−0.5566269D+01	0.2200686D+01	0.4523067D+01

Table 2. The convergence of the results (NT = total number of unknowns)

χ	NT	K(SC)	K(BCC)	K(FCC)
1.0	12	41.12	142.3	348.3
	27	42.14	162.1	362.1
	37	42.07	163.6	424.8
	48	42.07	160.0	437.9
0.95	12	28.6	-	104.0
	27	27.7	76.3	150.0
	37	27.9	78.7	145.1
	48	27.9	78.7	152.3
0.90	12	19.22	-	67.00
	27	19.16	42.8	65.13
	37	19.16	42.8	65.16
0.85	12	13.65	-	-
	37	13.64	25.81	34.6
	48	13.64	25.81	34.6

Table 3. The dimensionless drag K for three cubic arrays

	SC		BCC		FCC	
χ	K (converged)	K (Eq.60)	K (converged)	K (Eq.60)	K (converged)	K (Eq.60)
0.1	1.1646	1.1646	1.1861	1.1861	1.1924	1.1924
0.2	1.3881	1.3881	1.4487	1.4487	1.4669	1.4669
0.3	1.7000	1.7000	1.8331	1.8331	1.8741	1.8741
0.4	2.1518	2.1518	2.4234	2.4234	2.5103	2.5103
0.5	2.8420	2.8420	3.887	3.3836	3.5748	3.5748
0.6	3.9738	3.9738	5.1083	5.1083	5.5376	5.5376
0.7	6.004	6.004	8.565	8.565	9.717	9.717
0.8	10.05	10.06	16.9	16.851	20.9	20.8
0.85	13.64	13.71	25.8	25.8	34.6	34.2
0.90	19.16	19.5	42.8	42.5	65.1	61.9
0.95	27.9	29.8	78.7	76.8	152	125.1
1.0	42.1	50.7	162±2	153.6	438±10	283.3

functions to represent these solutions, as well as with the value $k = 42.5$ determined experimentally by Martin *et al.* (1951). In figure 1 the above results from the direct substitution method are given as a function of c. Also shown by dashed curves are the predictions from the series [1] and [49].

Body- and face-centered cubic arrays

The results for these cubic arrays are also given in tables 1 to 3. Here the series solution for K at $\chi = 1$ has not converged as yet, however, unlike the case for the simple cubic array, oscillations are absent, at least, up to $s = 30$. Once again, the direct substitution method converged rapidly. Our results for body-centered cubic arrays agree with those of Zick & Homsy (1981), who reported the value $K = 163$ for $\chi = 1$, as well as the value $K = 170$ found experimentally by Susskind & Becker (1967) for $\chi = 1$.

For the face-centered cubic arrays our results converged rapidly for $\chi \leq 0.95$. For χ equal to unity, however, the convergence is slow as seen in table 2 which lists the computed values of K for $N \leq 3$. Unfortunately, round-off errors in the computations become significant for N greater than 3 and therefore a more accurate estimate for K was not obtained. At any rate, with $N = 3$ the value $K = 438$ computed here agrees well with the values $K = 435$ reported by Zick & Homsy (1981) and $K = 398$ found experimentally by Martin *et al.* (1951).

The values thus calculated of K for closely packed cubic arrays allow us to obtain an estimate for the drag on a sphere in a closely packed random array if we assume that K depends only on c_{max} at $\chi = 1$. As mentioned by Batchelor & O'Brien (1977) c_{max} is approximately 0.62 for a random array of equal-sized spheres. Recalling that K equals 42, 162, and 438 for, respectively, simple, body-centered and face-centered cubic arrays for which the corresponding values of c_{max} are 0.52, 0.68 and 0.74, we find by interpolation that $K \sim 87$ for $c_{max} = 0.62$. This is in close agreement with the value $K = 94$, obtained by applying the well-known Blake–Kozeny correlation

$$K = \frac{25\, c_{max}}{3(1 - c_{max})^3} \text{ at } c_{max} = 0.62.$$

5. THE TWO-DIMENSIONAL ARRAYS

The problem of slow flow through an array of infinitely long circular cylinders with their axes parallel to x_3-axis can be treated in a similar manner (Hasimoto, 1959). We consider here square and hexagonal arrays and assume that the mean flow is in the x_1-direction. The components of velocity in this case are given by

$$u_1 = U_0 - \frac{1}{4\pi}\left[\mathbf{G}\left(S_1 - \frac{\partial^2 S_2}{\partial x_1^{\,2}}\right) + \mathbf{H}\frac{\partial^2 S_1}{\partial x_1^{\,2}}\right], \qquad [62]$$

$$u_2 = \frac{1}{4\pi}\left[G\frac{\partial^2 S_2}{\partial x_1 \partial x_2} - H\frac{\partial^2 S_1}{\partial x_1 \partial x_2}\right], \qquad [63]$$

where the differential operators $\mathbf{G}$ and $\mathbf{H}$ are

$$\mathbf{G} = \sum_{n=0}^{\infty} A_n \frac{\partial^{2n}}{\partial x_1^{\,2n}}, \qquad [64]$$

$$\mathbf{H} = \sum_{n=0}^{\infty} B_n \frac{\partial^{2n}}{\partial x_1^{\,2n}}. \qquad [65]$$

In order to determine A_n and B_n we expand S_1 and S_2 near $r = 0$

$$S_1 = -2\ln r - c_1 + \frac{\pi r^2}{\tau_0} + \sum_{n=2}^{\infty} a_n r^{2n} \cos 2n\theta. \qquad [66]$$

$$S_2 = \frac{1}{2} r^2(1 - \ln r) + c_2 - \frac{c_1 r^2}{4} + \frac{\pi r^4}{16\tau_0} + \sum_{n=2}^{\infty} (\tilde{a}_n r^2 + b_n) r^{2n} \cos 2n\theta \qquad [67]$$

where

$$r = (x_1^{\,2} + x_2^{\,2})^{1/2}, \quad \theta = \tan^{-1}(x_1/x_2), \qquad [68]$$

and

$$\tilde{a}_n = a_n/4(2n+1). \qquad [69]$$

Also, it can be shown that the coefficients a_n and b_n are given by:

$$a_n = \frac{1}{2^{2n-1}(2n)!}\left[G e^{2n}\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}\right)\{S_1 + 2\ln r\}\right]_{r=0} \qquad [70]$$

$$b_n = \frac{1}{2^{2n-1}(2n)!}\left[Ge^{2n}\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}\right)\left\{S_2 + \frac{1}{2}r^2 \ln r\right\}\right]_{r=0} \quad [71]$$

where

$$Ge^n(x_1, x_2) = r^n \cos n\theta. \quad [72]$$

Following a treatment analogous to that of the three-dimensional case, we find that the magnitude $F'/\mu U$, the dimensionless drag force per unit length of a cylinder, equals $4\pi A_0$ and

$$U_0 = 1 + \frac{B_0}{\tau_0} \quad [73]$$

Substituting the expressions [66] and [67] for S_1 and S_2 into [62] and [63] and equating to zero the coefficients of Ge^0, Ge^2, Ge^4 in u_1 and of $\sin 2\theta$ in u_2 we obtain four equations in the four unknowns A_0, A_1, B_0, B_1 which when solved yield

$$\frac{4\pi\mu U}{F'} = -\ln a - \frac{c_1}{2} + \frac{\pi a^2}{\tau_0} - \left(\frac{\pi^2}{4\tau_0} + 24^2 b_2^2\right) a^4 - 384\, a_2 b_2 a^6 + 0(a^8). \quad [74]$$

The basic vectors and the constants c_1, a_2, and b_2 for the square and the hexagonal arrays are given in appendix 1. On substituting these constants into (74) we obtain

$$\frac{4\pi\mu U}{F'} = \begin{cases} -\frac{1}{2}\ln c - 0.738 + c - 0.887\, c^2 + 2.039\, c^3 + 0(c^4) \text{ (square array)}, \\ -\frac{1}{2}\ln c - 0.745 + c - \frac{1}{4}c^2 + 0(c^4) \text{ (hexagonal array)}, \end{cases} \quad [75]$$

with

$$c = \pi a^2/\tau_0. \quad [76]$$

We see that to $0(c)$, [75] agrees with Hasimoto's result [3].

Recently, the present authors (1982a) calculated F' via a numerical solution of the Stokes equation for the complete range of c for these two arrays. On comparing with these numerical results we find that [75] provides an estimate of F' to within 5% for $c < 0.3$.

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APPENDIX 1: THE BASIC VECTORS AND THE CONSTANTS OF THE REGULAR ARRAYS OF SPHERES AND CYLINDERS.

Cubic arrays

(1) *The basic vectors.* The basic vectors and τ_0 for the cubic arrays are (Hasimoto (1959)):

(i) Simple cubic array

$$\left.\begin{matrix}\mathbf{a}_{(1)}\\ \mathbf{a}_{(2)}\\ \mathbf{a}_{(3)}\end{matrix}\right\} = \left\{\begin{matrix}(1,0,0)\\ (0,1,0)\\ (0,0,0)\end{matrix}\right\}, \quad \tau_0 = 1, \quad \left.\begin{matrix}\mathbf{b}_{(1)}\\ \mathbf{b}_{(2)}\\ \mathbf{b}_{(3)}\end{matrix}\right\} = \left\{\begin{matrix}(1,0,0)\\ (0,1,0)\\ (0,0,1)\end{matrix}\right\}, \tag{A.1}$$

(ii) Body-centered cubic array

$$\left.\begin{matrix}\mathbf{a}_{(1)}\\ \mathbf{a}_{(2)}\\ \mathbf{a}_{(3)}\end{matrix}\right\} = \frac{1}{2}\left\{\begin{matrix}(1,1,-1)\\ (-1,1,1)\\ (1,-1,1)\end{matrix}\right\}, \quad \tau_0 = \frac{1}{2}, \quad \left.\begin{matrix}\mathbf{b}_{(1)}\\ \mathbf{b}_{(2)}\\ \mathbf{b}_{(3)}\end{matrix}\right\} = \left\{\begin{matrix}(1,1,0)\\ (0,1,1)\\ (1,0,1)\end{matrix}\right\}. \tag{A.2}$$

(iii) Face-centered cubic array

$$\left.\begin{matrix}\mathbf{a}_{(1)}\\ \mathbf{a}_{(2)}\\ \mathbf{a}_{(3)}\end{matrix}\right\} = \frac{1}{2}\left\{\begin{matrix}(1,1,0)\\ (0,1,1)\\ (1,0,1)\end{matrix}\right\}, \quad \tau_0 = \frac{1}{4}, \quad \left.\begin{matrix}\mathbf{b}_{(1)}\\ \mathbf{b}_{(2)}\\ \mathbf{b}_{(3)}\end{matrix}\right\} = \left\{\begin{matrix}(1,1,-1)\\ (-1,1,1)\\ (1,-1,1)\end{matrix}\right\}. \tag{A.3}$$

(2) *Evaluation of the constants $\bar{c}$, a_{lm} and b_{lm}.* As shown by Hasimoto (1959)

$$\bar{c} = \frac{2}{\sqrt{\alpha}} + \frac{\alpha}{\tau_0} - \frac{1}{\sqrt{\alpha}}\sum_{n\neq 0}\phi_{-1/2}\left(\frac{\pi r_n^2}{\alpha}\right) - \frac{\alpha}{\tau_0}\sum_{k_n\neq 0}\phi_0(\pi\alpha k_n^2), \tag{A.4}$$

$$\left.\begin{matrix}a_{lm}\\ b_{lm}\end{matrix}\right\} = \frac{\epsilon_m 2^{2l}(2l)!(2l-4m)!}{(4l)!(2l+4m)!}\left[Y_{2l}^{4m}\left(\frac{\partial}{\partial x_1},\frac{\partial}{\partial x_2},\frac{\partial}{\partial x_3}\right)\left\{\begin{matrix}S_1 - \dfrac{1}{r}\\ S_2 - \dfrac{r}{2}\end{matrix}\right\}\right]_{r=0} \tag{A.5}$$

$$(\epsilon_0 = 1,\ \epsilon_m = 2 \text{ for } m > 0),$$

where the constant α must be chosen so as to facilitate the subsequent calculations (the constant $\bar{c}$, of course, is independent of α) and $\phi_\nu(x)$ is the incomplete gamma function

$$\phi_\nu(x) = \int_1^\infty e^{-x\xi}\,\xi^\nu\,d\xi. \qquad [A.6]$$

Further, $\phi_\nu(x)$ satisfies the recurrence relations

$$\phi_\nu' = -\phi_{\nu+1}, \quad x\phi_\nu = e^{-x} + \nu\phi_{\nu-1} \qquad [A.7]$$

with

$$\phi_0(x) = e^{-x}/x, \quad \phi_{-1/2}(x) = \frac{\sqrt{\pi}}{\sqrt{x}}\,\mathrm{erfc}(\sqrt{x}). \qquad [A.8]$$

Using [A.7] and [A.8], ϕ's were calculated accurately to at least ten significant digits. Now, the constants a_{lm} and b_{lm} can be evaluated from [A.5] using two different methods. The first method to be described below was used for $l \leq 8$ whereas the second was used for other values of l.

(i) *Ewald's technique.* Again, as shown by Hasimoto (1959)

$$\sum_{k_n \neq 0} \frac{e^{-2\pi i(\mathbf{k_n}\cdot\mathbf{r})}}{k_\mathbf{n}^{2m}} = \frac{\pi^m \alpha^m}{(m-1)!}\left[\tau_0\alpha^{-3/2+\lambda}\sum_\mathbf{n}\phi_{-m+\lambda}\left(\frac{\pi(\mathbf{r}-\mathbf{r}_n)^2}{\alpha}\right) - \frac{1}{m}\right.$$
$$\left. + \sum_{\mathbf{k_n}\neq 0} e^{-2\pi i(\mathbf{k_n}\cdot\mathbf{r})}\,\phi_{m-1}(\pi\alpha k_\mathbf{n}^2)\right], \qquad [A.9]$$

where

$$\lambda = \begin{cases} \frac{1}{2} & \text{for the array of spheres} \\ 0 & \text{for the array of cylinders.} \end{cases} \qquad [A.10]$$

Substituting for S_1 and S_2 obtained from [A.9] into [A.5] and simplifying we obtain

$$\bar{a}_{lm} = \frac{\alpha(2\pi)^{2l}}{\tau_0}\left[\tau_0\alpha^{-(3/2)-2l}\sum_{\mathbf{n}\neq 0} Y_{2l}^{4m}(x_{1\mathbf{n}}, x_{2\mathbf{n}}, x_{3\mathbf{n}})\,\phi_{2l-1/2}\left(\frac{\pi r_\mathbf{n}^2}{\alpha}\right)\right.$$
$$\left. + \sum_{\mathbf{k_n}\neq 0} Y_{2l}^{4m}(k_{1\mathbf{n}}, k_{2\mathbf{n}}, k_{3\mathbf{n}})\phi_0(\pi\alpha k_\mathbf{n}^2)\right], \qquad [A.11]$$

$$\bar{b}_{lm} = \frac{-\alpha^2(2\pi)^{2l}}{4\pi\tau_0}\left[\tau_0^{-(3/2)-2l}\sum_{n\neq 0}\phi_{2l-(3/2)}\left(\frac{\pi r_\mathbf{n}^2}{\alpha}\right) Y_{2l}^{4m}(x_{1\mathbf{n}}, x_{2\mathbf{n}}, x_{3\mathbf{n}})\right.$$
$$\left. + \sum_{\mathbf{k_n}=0}\phi_0(\pi\alpha k_\mathbf{n}^2)\,Y_{2l}^{4m}(k_{1\mathbf{n}}, k_{2\mathbf{n}}, k_{3\mathbf{n}})\right], \qquad [A.12]$$

where

$$\bar{a}_{lm} = \frac{(2l+4m)!}{\epsilon_m(2l-4m)!}\,a_{lm} \quad \text{and} \quad \bar{b}_{lm} = \frac{(2l+4m)!}{\epsilon_m(2l-4m)}\,b_{lm}.$$

The sums in the above equation converge very rapidly. Thus $\bar{a}_{lm}$ and $\bar{b}_{lm}$ $(l \le 8)$ could be determined to seven significant digits with $|\mathbf{n}| \le 5$. For $l > 8$, however, the incomplete gamma functions could not be evaluated with sufficient accuracy.

(ii) ***The direct sum method.*** Using [25] and the fact that the average values of S_1 over a unit cell is zero, it can be shown that

$$S_1(\mathbf{r}) = \lim_{N\to\infty}\left[\sum_{\mathbf{n}}^{|\mathbf{n}|\le N}\left\{\frac{1}{|\mathbf{r}-\mathbf{r}_\mathbf{n}|} - \frac{1}{\tau_0}\int_{\tau_\mathbf{n}}\frac{d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\right\}\right] \qquad \text{A.13]}$$

where $\tau_\mathbf{n}$ is the unit cell situated at $\mathbf{r}_\mathbf{n}$ except for the unit cell containing $\mathbf{r}$. A sphere of radius $\epsilon(\epsilon \to 0)$ is excluded from $\tau_\mathbf{n}$ in that case. Substituting [A.13] into [A.5] and simplifying we obtain

$$\bar{a}_{lm} = \lim_{N\to\infty}\sum_{|\mathbf{n}|\ne 0}^{|\mathbf{n}|\le N}\frac{Y_{2l}^{4m}(x_{1\mathbf{n}}, x_2\mathbf{n}, x_{3\mathbf{n}})}{r_\mathbf{n}^{4l+1}}. \qquad [A.14]$$

Similarly it can be shown that

$$\bar{b}_{lm} = \frac{-1}{2(4l-1)}\left\{\lim_{N\to\infty}\sum_{|\mathbf{n}|\ne 0}^{|\mathbf{n}|\le N}\frac{Y_{2l}^{4m}(x_{1\mathbf{n}}, x_{2\mathbf{n}}, x_{3\mathbf{n}})}{r_\mathbf{n}^{4l-1}}\right\}. \qquad [A.15]$$

Note that the above expression for a_{l0} is identical to the sum S_{2l} in Rayleigh's (1892) theory on the effective conductivities of composite materials consisting of cubic array of spheres plus a continuous homogeneous matrix of different conductivity. [A14] and [A.15] are particularly useful for determining $\bar{a}_{lm}$ and $\bar{b}_{lm}$ when l is large.

The first few values of $\bar{a}_{lm}$, $\bar{b}_{lm}$ and $\bar{c}$ are listed in table 4. As mentioned earlier, for $l > 8$, the direct sum method was employed exclusively. In fact, this method gives fairly accurate results even for smaller values of l. Thus, we have also calculated a_{l0} and b_{l0}'s for l between 4 and 8 and found that in this range both methods agreed to at least five significant digits.

Table 4. The computed values of the constants

	SC	BCC	FCC
$\bar{c}$	0.2837297D+1	0.3639233D+1	0.4584862D+1
a_{20}	0.3108227D+1	-0.3106460D+1	-0.7525692D+1
a_{30}	0.5733293D+0	0.5446557D+1	-0.2663489D+2
a_{40}	0.3259293D+1	0.7648391D+1	0.8118646D+2
$\bar{a}_{41}$	0.5475612D+4	0.1284930D+5	0.1363932D+6
$\bar{a}_{42}$	0.8541849D+7	0.2004490D+8	0.2127735D+9
a_{50}	0.1009224D+1	-0.9396657D+1	-0.1524345D+1
$\bar{a}_{51}$	-0.1119028D+5	0.1041901D+6	0.1690194D+5
$\bar{a}_{52}$	-0.6848449D+8	0.6376436D+9	0.1034399D+9
b_{20}	-0.1945688D+0	0.1199684D+0	0.2133181D+0
b_{30}	-0.1966601D-1	-0.1862257D+0	0.5825414D+0
b_{40}	-0.1145416D+0	-0.2197556D+0	-0.1384665D+1
$\bar{b}_{41}$	-0.1924301D+3	-0.3691894D+3	-0.2326242D+4
$\bar{b}_{42}$	-0.3001910D+6	-0.5759355D+6	-0.3628937D+7
b_{50}	-0.2625465D-1	0.1787547D+0	-0.1577060D-2
$\bar{b}_{51}$	0.2911115D+3	-0.1982033D+4	0.1748615D+2
$\bar{b}_{52}$	0.1781602D+7	-0.1213004D+8	0.1070152D+6

McPhedran & McKenzie (1978) have also calculated a_{l0} for the simple cubic array. The values reported here are in complete agreement with those reported by these authors who evaluated these constants to five significant digits. Our values for b_{20} and $\bar{c}$ agree with Hasimoto's (1959) except for the simple cubic array where, as pointed out by Zuzovski (1976), the value of b_{20} stated by Hasimoto has a sign error.

Two-dimensional arrays

(1) *The basic vectors.* (i) Square array

$$\left.\begin{matrix}\mathbf{a}_{(1)}\\ \mathbf{a}_{(2)}\end{matrix}\right\} = \left\{\begin{matrix}(1,0)\\ (0,1)\end{matrix}\right\}, \tau_0 = 1, \quad \left.\begin{matrix}\mathbf{b}_{(1)}\\ \mathbf{b}_{(2)}\end{matrix}\right\} = \left\{\begin{matrix}(1,0)\\ (0,1)\end{matrix}\right\}. \qquad [A.16]$$

(ii) Hexagonal array

$$\left.\begin{matrix}\mathbf{a}_{(1)}\\ \mathbf{a}_{(2)}\end{matrix}\right\} = \left\{\begin{matrix}(1,0)\\ \frac{1}{2}, \frac{\sqrt{3}}{2}\end{matrix}\right\}, \tau_0 = \frac{\sqrt{3}}{2}, \quad \left.\begin{matrix}\mathbf{b}_{(1)}\\ \mathbf{b}_{(2)}\end{matrix}\right\} = \left\{\begin{matrix}1, \frac{-1}{\sqrt{3}}\\ 0, \frac{2}{\sqrt{3}}\end{matrix}\right\}. \qquad [A.17]$$

(2) *The constants c_1, a_2, and b_2.* The constant c_1 is given by (Hasimoto (1959))

$$c_1 = \gamma + \ln\frac{\pi}{\alpha} + \frac{\alpha}{\tau_0} - \sum_{\mathbf{n}\neq 0} \phi_{-1}\left(\frac{\pi r_{\mathbf{n}}^2}{\alpha}\right) - \frac{\alpha}{\tau_0}\sum_{\mathbf{k}_{\mathbf{n}}=0} \phi_0(\pi\alpha k_{\mathbf{n}}^2), \qquad [A.18]$$

where $\gamma = 0.577215\ldots$ is Euler's constant.

Following a treatment analogous to that for the three dimensional case, we find that

$$a_l = \frac{\alpha(2\pi)^{2l}}{2^{2l-1}(2l)!\tau_0}\left[\tau_0\,\alpha^{-1-2l}\sum_{\mathbf{n}\neq 0} Ge^{2l}(x_{1\mathbf{n}}, x_{2\mathbf{n}})\,\phi_{-1+2l}\left(\frac{\pi r_{\mathbf{n}}^2}{\alpha}\right)\right.$$

$$\left.\sum_{\mathbf{k}_{\mathbf{n}}\neq 0} Ge^{2l}(k_{1\mathbf{n}}, k_{2\mathbf{n}})\phi_0(\pi\alpha k_{\mathbf{n}}^2)\right]. \qquad [A.19]$$

$$b_l = \frac{-\alpha^2(2\pi)^{2l}}{\pi\tau_0 2^{2l+1}(2l)!}\left[\tau_0\alpha^{-1-2l}\sum_{\mathbf{n}} \mathrm{Ge}^{2l}(x_{1\mathbf{n}}, x_{2\mathbf{n}})\,\phi_{-2+2l}\left(\frac{\pi r_{\mathbf{n}}^2}{\alpha}\right)\right.$$

$$\left. + \sum_{\mathbf{k}_{\mathbf{n}}=0} Ge^{2l}\,(k_{1\mathbf{n}}, k_{2\mathbf{n}})\phi_1(\pi\alpha k_{\mathbf{n}}^2)\right].$$

The computed values are (i) Square array

$$\begin{cases} c_1 = 2.621 & \text{(Hasimoto (1959))} \\ a_2 = 1.576. \\ b_2 = 1.664 \end{cases} \qquad [A.21]$$

(ii) Hexagonal array

$$\begin{cases} c_1 = 2.779 \\ a_2 = b_2 = 0^{\cdot} \end{cases} \qquad [A.22]$$

In fact, as shown by Perrins *et al.* (1979) due to symmetry, $a_n = b_n = 0$ for all n not divisible by 3.

APPENDIX 2: RESULTS ON THE DIFFERENTIATION OF THE VARIOUS TERMS IN S_1 AND S_2

The following results for spherical harmonics are taken from Hobson (1937), p. 138

$$\frac{\partial^{n-m}}{\partial x_1{}^{n-m}}\left[\left(\frac{\partial}{\partial \xi}\right)^m+\left(\frac{\partial}{\partial \eta}\right)^m\right]\frac{1}{r}=\frac{(-1)^{n-m}(n-m)!}{2^{m-1}r^{2n+1}}\,Y_n{}^m, \quad \text{[A.23]}$$

$$\frac{\partial^k}{\partial x_1{}^k}\left[\left(\frac{\partial}{\partial \xi}\right)^\lambda+\left(\frac{\partial}{\partial \eta}\right)^\lambda\right]Y_n{}^m=B\,Y^{|m-\lambda|}_{n-\lambda-k}+\frac{1}{2^\lambda}\frac{(n+m)!}{(n+m-k)!}\,Y^{\lambda+m}_{n-\lambda-k}, \quad \text{[A.24]}$$

where

$$B=\begin{cases}\dfrac{(-1)^\lambda}{2^\lambda}\dfrac{(n+m)!}{(n+m-2\lambda-k)!}\text{ for } \lambda\le m\\[2ex] \dfrac{(-1)^m}{2^\lambda}\dfrac{(n+m)!}{(n-m-k)!}\text{ for } \lambda> m.\end{cases} \quad \text{[A.25]}$$

Further, using the theorem stated by Hobson (1937), p. 127

$$f_n\left(\frac{\partial}{\partial x_1},\frac{\partial}{\partial x_2},\frac{\partial}{\partial x_3}\right)F(r^2)=\left\{2^n\frac{\mathrm{d}^nF}{\mathrm{d}(r^2)^n}+\frac{2^{n-2}}{1!}\frac{\mathrm{d}^{n-1}F}{\mathrm{d}(r^2)^{n-1}}\nabla^2+\cdots\right\}f_n(x_1,x_2,x_3) \quad \text{[A.26]}$$

where f_n is a homogeneous polynomial of degree n in x_1, x_2 and x_3 and taking $F(r^2)=r$, it can be shown that

$$\left(\frac{\partial}{\partial x_1}\right)^{n-m}\left[\left(\frac{\partial}{\partial \xi}\right)^m+\left(\frac{\partial}{\partial \eta}\right)^m\right]r=\frac{(-1)^{n-m}(n-m)!}{2^{m-1}(2n-1)}\left[\frac{Y^m_{n-2}}{r^{2n-3}}-\frac{Y_n{}^m}{r^{2n-1}}\right]. \quad \text{[A.27]}$$

In deriving [A.27] use has also been made of the series representation for the spherical harmonics (Hobson (1937), p. 137)

$$Y_n{}^m=\frac{(-1)^m(2n)!}{2^{n+1}n!(n-m)!}(\xi^m+\eta^m)\left(x_1^{n-m}-\frac{(n-m)(n-m-1)}{2(2n-1)}r^2x_1+\cdots\right). \quad \text{[A.28]}$$

The above series representation can also be employed to derive the formulae:

$$\left(\frac{\partial}{\partial x_1}\right)^{n-m-p}\left[\left(\frac{\partial}{\partial \xi}\right)^m+\left(\frac{\partial}{\partial \eta}\right)^m\right]\left[\left(\frac{\partial}{\partial \xi}\right)^p+\left(\frac{\partial}{\partial \eta}\right)^p\right]\left(\frac{1}{r}\right)$$

$$=\frac{1}{r^{2n+1}}\left\{\frac{(-1)^{n-m-p}(n-m-p)!}{2^{m+p-1}}\,Y_n^{m+p}+\frac{(-1)^{n-m}(n-m+p)!}{2^{m+p-1}}\,Y_n^{m-p}\right\}(m\geqslant p), \quad \text{[A.29]}$$

$$\frac{\partial^k}{\partial x_1{}^k}(r^2Y_n{}^m)=\frac{(n+m)!}{(n+m-k)!}\frac{(4n+6)}{(4n+6-4k)}r^2\,Y^m_{n-k}$$

$$+\frac{(n+m)!}{(n+m+2-k)!}\left\{\frac{(n-m+2)!}{(n-m)!}-\frac{(4n+6)(n+2-m-k)!}{(4n+6-4k)(n-m-k)!}\right\}Y^m_{n-k+2} \quad \text{[A.30]}$$

$$\left[\left(\frac{\partial}{\partial \xi}\right)^{\lambda}+\left(\frac{\partial}{\partial \eta}\right)^{\lambda}\right](r^2 Y_n^m) = A r^2\, Y_{n-\lambda}^{|\lambda-m|} + B\, Y_{n+2-\lambda}^{|\lambda-m|}$$

$$+\frac{1}{2^{\lambda}}\frac{4n+6}{4n+6-4\lambda} r^2\, Y_{n-\lambda}^{m+\lambda} - \frac{\lambda(n+m)!}{2^{\lambda-2}(n+m+2)!}\left\{m+\lambda+\frac{(n+2-m-2\lambda)!}{(n-m-2\lambda)!}\frac{1}{4n+6-4\lambda}\right\} Y_{n+2-\lambda}^{m+\lambda}, \qquad [A.31]$$

where

$$A=\begin{cases}\dfrac{(-1)^{\lambda}(n+m)!}{2^{\lambda}(n+m-2\lambda)!}\dfrac{(4n+6)}{(4n+6-4\lambda)} & \text{for } m \geq \lambda \\ \dfrac{(-1)^{m}(n+m)!}{2^{\lambda}(n-m)!}\dfrac{(4n+6)}{(4n+6-4\lambda)} & \text{for } m < \lambda,\end{cases} \qquad [A.32]$$

$$B=\begin{cases}\dfrac{(-1)^{\lambda}(n+m)!(n+2-m)!(-4\lambda)}{2^{\lambda}(n+m+2-2\lambda)!(n-m)!(4n+6-4\lambda)} & \text{for } m \geq \lambda \\ \dfrac{(-1)^{m}(n+m)!(-4\lambda)}{2^{\lambda}(n+2-m)!}\left\{(\lambda-m)+\dfrac{(n+2+m-2\lambda)!}{(n+m-2\lambda)!(4n+6-4\lambda)}\right\} & \text{for } \lambda > m.\end{cases} \qquad [A.33]$$

In above relations, the coefficient of Y_n^m must be set equal to zero for $m > n$.