# Microstructure functions for random media with impenetrable particles

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We introduce a model consisting of nonaligned and impenetrable particles. This model is obtained by placing particles of random orientation within ''security spheres,'' typically chosen to be spheres in thermal equilibrium. The particles in general are allowed to be nonspherical. We obtain an analytical expression for the function $S_n$, the probability that $n$ points simultaneously lie outside of the particle phase. This characterization of the microstructure appears in certain rigorous bounds on the effective properties of random materials. We also evaluate $S_2$ for various specific examples of this model, including nonaligned impenetrable ellipsoids. [S1063-651X(99)09811-6]

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## I. INTRODUCTION

Much progress has been made in recent years in characterizing the microstructure of statistically homogeneous two-phase random media via a variety of $n$-point correlation functions [1–4]. This microstructural information is fundamental in rigorously determining the effective transport, electromagnetic and mechanical properties of ergodic two-phase random media [5–11]. One commonly used function in this regard is the $n$-point phase probability function $S_n(\mathbf{x}^n)$, which is the probability that $n$ points in configuration $\mathbf{x}^n \equiv \mathbf{x}_1, \ldots, \mathbf{x}_n$ all lie in one of the phases (say, phase 1). We may explicitly write this function as

$$S_n(\mathbf{x}_n) = \left\langle \prod_{i=1}^{n} I(\mathbf{x}_i) \right\rangle \tag{1}$$

where $I(\mathbf{x})$ is the indicator function for phase 1. For particulate models, phase 1 is typically defined to be the void phase, while phase 2 is defined to be the particle phase. This microstructure function has been studied for totally impenetrable spheres [12,13], allowing for evaluation of rigorous bounds on the effective properties [14,15]. These bounds have also been numerically evaluated for various random media by the fast multipole method [11,16,17]. More recently, this analytical approach has been applied to the nonparticulate model of level cuts of Gaussian random fields [18,19].

Using spheres as particles makes possible the simplification of certain complicated integrals in these bounds. However, allowing the particles to be nonspherical introduces a significant extra level of complexity. If the positions of the nonspherical particles are determined by a Poisson process (i.e., the particles are fully penetrable), then this model may be handled by the theoretical techniques for Boolean models [20]. Much less is known if the particles are not permitted to overlap; even mathematically defining such models is problematic. The microstructure and effective properties of oriented ellipsoids [21,22] have been studied through a transformation of a system of hard spheres by stretching or compressing one of the coordinate axes. More recently, the simulation of nonaligned nonspherical particles through a complicated algorithm of random sequential addition has been considered [23].

The model of impenetrable particles considered in this paper consists of particles with *arbitrary* fixed shape and *random* orientation. This model is generated by placing the particles within *security spheres* of unit radius. We choose the security spheres to be generated by a system in thermal equilibrium. The particles are placed at random orientations which are independent of each other and of the locations of the centers of the security spheres. A realization of this model is shown in Fig. 1. In this figure, the security spheres (in two dimensions, circles) have a volume fraction of $\phi_2^s$

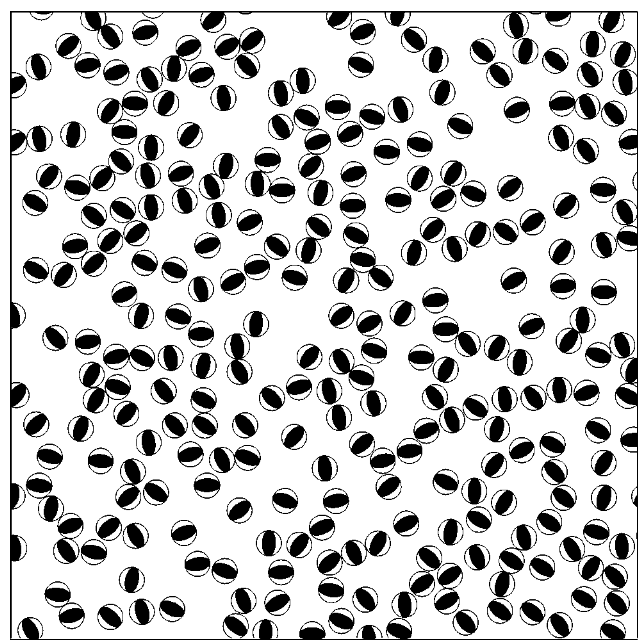

FIG. 1. A two-dimensional system of impenetrable particles of arbitrary fixed shape and random orientation. The particles (filled) are placed within impenetrable security spheres (outlined), which we choose to be generated by a system of hard spheres in thermal equilibrium. The particles are then randomly oriented with the security spheres.

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$=0.35$, and the particles are ellipses with semimajor axis 1 and semiminor axis 0.5. The volume fraction of the particles is thus $\phi_2=0.175$.

This model has one shortcoming: it does not permit all possible arrangements of totally impenetrable particles. In the above example, requiring the centers of ellipses to be separated by at least the length of major axis is significantly more restrictive than simply requiring the ellipses to be nonoverlapping. Nevertheless, we see from Fig. 1 that we may obtain a nontrivial arrangement of nonaligned particles with this model.

Requiring the particles to be randomly aligned within security spheres introduces a certain probabilistic spherical symmetry in this model, permitting the evaluation of the microstructure functions. In Sec. II, we present a general expression for $S_n$ for impenetrable particles within security spheres. We also simplify this general expression for $S_1$, $S_2$, and $S_3$, discussing the efficient numerical evaluation of $S_2$. In Section III, we evaluate $S_2$ for two examples of this model: impenetrable spherical cores and randomly aligned ellipsoids.

## II. ANALYTICAL EXPRESSION FOR $S_n$

For systems of impenetrable spheres of unit radius, Torquato and Stell [12] have evaluated the $n$-point matrix probability function as

$$S_n(\mathbf{x}^n)=1+\sum_{s=1}^{n}\frac{(-1)^s}{s!}\int \rho_s(\mathbf{x}_{n+1},\ldots,\mathbf{x}_{n+s})\times\prod_{j=n+1}^{n+s}\left[1-\prod_{i=1}^{n}\{1-m(\mathbf{x}_{ij})\}\right]d\mathbf{x}_{n+j}. \quad (2)$$

This series truncates at the $n$th term because the particles are not permitted to overlap. In this expression, the function $\rho_s(\mathbf{x}^s)$ is the probability density function for finding $s$ particle centers with configuration $\mathbf{x}^s$. Also, the function $m$ is the indicator function for one sphere; that is,

$$m(\mathbf{x})=\begin{cases}1, & |\mathbf{x}|<1\\ 0, & |\mathbf{x}|\geqslant 1.\end{cases} \quad (3)$$

We will slightly abuse notation and write this function as $m(x)$ when the direction of $\mathbf{x}$ is unimportant. Also, the points $\mathbf{x}_{n+1},\ldots,\mathbf{x}_{n+s}$ may be considered as ''test'' particle centers, and

$$\mathbf{x}_{ij}=|\mathbf{x}_i-\mathbf{x}_j|. \quad (4)$$

In this paper, we are concerned not with impenetrable spheres but with particles within the spheres. Let particle $j$ be contained within the sphere with center $\mathbf{x}_j$ with some given orientation $\omega_j$. Then we have the following expression for $S_n$:

$$S_n(\mathbf{x}^n;\Omega)=1+\sum_{s=1}^{n}\frac{(-1)^s}{s!}\int \rho_s(\mathbf{x}_{n+1},\ldots,\mathbf{x}_{n+s})\times\prod_{j=n+1}^{n+s}\left[1-\prod_{i=1}^{n}\{1-m(\mathbf{x}_{ij};\omega_j)\}\right]d\mathbf{x}_{n+j}, \quad (5)$$

where $m(\cdot\,;\omega_j)$ is the indicator function for a particle with orientation $\omega_j$. The argument $\Omega$ above represents all of the given orientations of the particles. We assume that the $\omega_j$ are independent and identically distributed, uniformly over all possible orientations. We also assume that the $\omega_j$ are independent of the positions of the security spheres.

The above expression is only valid if the orientations of the particles are deterministically specified. If the particles are instead randomly oriented within the spheres, we may calculate $S_n$ by first taking the *conditional* expectation of $S_n(\mathbf{x}^n;\Omega)$, conditioned on the orientations of the particles. Using the expectation of conditional expectations, we conclude that

$$S_n(\mathbf{x}^n)=E[E\{S_n(\mathbf{x}^n;\Omega)|\Omega\}]. \quad (6)$$

Using (5), this simplifies to the final expression

$$S_n(\mathbf{x}^n)=1+\sum_{s=1}^{n}\frac{(-1)^s}{s!}\int \rho_s(\mathbf{x}_{n+1},\ldots,\mathbf{x}_{n+s})\times E\left[\prod_{j=n+1}^{n+s}\left(1-\prod_{i=1}^{n}\{1-m(\mathbf{x}_{ij};\omega_j)\}\right)\right]d\mathbf{x}_{n+j}. \quad (7)$$

We now consider the simplification of this general expression for $S_1$, $S_2$, and $S_3$.

### A. Evaluation of $S_1$

To find the probability that one point lies outside of the particles, we substitute $n=1$ into the general expression (7). We find that

$$S_1(\mathbf{x}_1)=1-\int \rho_1(\mathbf{x}_2)E[m(x_{12};\omega_2)]d\mathbf{x}_2=1-\rho V_1, \quad (8)$$

where $V_1$ is the volume of a single particle and $\rho$ is the number density of the particles (and hence also the security spheres). This result is expected: the volume fraction of the security spheres is

$$\phi_2^s=\frac{4\pi\rho}{3}, \quad (9)$$

and hence the volume fraction of the particles is

$$\phi_2=\frac{\phi_2^s V_1}{4\pi/3}=\rho V_1. \quad (10)$$

### B. Simplification and evaluation of $S_2$

For impenetrable spheres, Torquato and Stell [12] simplified the general series expansion (2) for $S_2$ and $S_3$. We follow their technique to simplify $S_2$ and $S_3$ for the present model of particles within security spheres. If $n=2$, then (7) simplifies as

$$S_2(\mathbf{x}_1,\mathbf{x}_2)=1-\rho\int (1-E[\{1-m(\mathbf{x}_{13};\omega_3)\}\times\{1-m(\mathbf{x}_{23};\omega_3)\}])d\mathbf{x}_3 + \frac{\rho^2}{2}\int\int g(r_{34})(1-E[\{1-m(\mathbf{x}_{13};\omega_3)\}\times\{1-m(\mathbf{x}_{23};\omega_3)\}])(1-E[\{1-m(\mathbf{x}_{14};\omega_4)\}\times\{1-m(\mathbf{x}_{24};\omega_4)\}])\,d\mathbf{x}_3\,d\mathbf{x}_4, \quad (11)$$

where $r_{ij}=|\mathbf{x}_{ij}|$ and $g(r)=\rho^2(r)/\rho^2$ is the radial distribution function for the particle centers. Because the particles are not permitted to overlap, many of the above terms vanish after expanding, and we obtain our final expression for $S_2$:

$$S_2(\mathbf{x}_1,\mathbf{x}_2)=1-\rho\mathcal{V}_2(x_{12}) + \rho^2\int\int \mu(x_{13})g(r_{34})\mu(x_{42})d\mathbf{x}_3\,d\mathbf{x}_4. \quad (12)$$

In this expression,

$$\mu(x)=E[m(x;\omega)] \quad (13)$$

is the probability that a point a distance $x$ from the center of a security sphere is inside of a randomly oriented particle. Also,

$$\mathcal{V}_2(x_{12})=E\left[\int m(x_{13};\omega_3)+m(x_{23};\omega_3) - m(\mathbf{x}_{13};\omega_3)m(\mathbf{x}_{23};\omega_3)d\mathbf{x}_3\right] \quad (14)$$

is the expected union volume of two *aligned* particles, averaged over all possible (common) orientations $\omega_3$. This may be rewritten as

$$\mathcal{V}_2(x_{12})=\int \{\mu(x_{13})+\mu(x_{23})-\mu_2(\mathbf{x}_{13},\mathbf{x}_{23})\}d\mathbf{x}_3. \quad (15)$$

The function $\mu$ may be interpreted as a *gray-scale* *m*-function within the security sphere. Likewise,

$$\mu_2(\mathbf{x}_{13},\mathbf{x}_{23})=E[m(\mathbf{x}_{13};\omega)m(\mathbf{x}_{23};\omega)] \quad (16)$$

may be considered a gray-scale function for the intersection of two aligned particles. This is in contrast to the above *m*-function (3) which appears in the expansion of $S_n$ for impenetrable spheres; this function deterministically assumes the values of 0 or 1, depending on whether a point is outside or inside the sphere.

Assuming that the geometrical quantity $\mathcal{V}_2$ can be obtained analytically, efficient numerical evaluation of $S_2$ rests solely on the double integral in (12). We do so by following Torquato and Stell [12]. We define the three-dimensional Fourier transform by

$$\tilde{f}(k)=\int f(r)e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=\frac{4\pi}{k}\int_0^\infty f(r)r\,\sin(kr)dr \quad (17)$$

if the function $f$ is spherically symmetric. The inverse Fourier transform is then given by

$$f(r)=\frac{1}{8\pi^3}\int \tilde{f}(k)e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=\frac{1}{2\pi^2 r}\int_0^\infty \tilde{f}(k)k\sin(kr)dk. \quad (18)$$

Following Torquato and Stell, we find that the double integral of (12) is given by

$$\int\int \mu(x_{13})g(r_{34})\mu(x_{42})d\mathbf{x}_3\,d\mathbf{x}_4=V_1^2+M(r_{12}), \quad (19)$$

where $V_1$ is the volume of one particle,

$$M(r)=\frac{1}{2\pi^2 r}\int_0^\infty \frac{\tilde{c}(k)}{1-\rho\tilde{c}(k)}\tilde{\mu}^2(k)k\,\sin(kr)dk \quad (20)$$

and $c$ is the direct correlation function, obtained by solving the Ornstein-Zernike equation (Ref. [24]).

The function $\mu(r)$ of course depends on the specific shape of the particles within the security spheres. We notice that $\mu(r)$ is spherically symmetric since it is an average over all possible orientations of the particles; therefore, $\tilde{\mu}(k)$ is also spherically symmetric.

The direct correlation function has been solved exactly for a system of hard (in our case, security) spheres exactly in the Percus-Yevick approximation; see [24] for details. We find that the Fourier transform of this direct correlation function is

$$\tilde{c}(k)=-\frac{4\pi}{k^3}\Big\{\lambda_1[\sin(2k)-2k\cos(2k)] + \frac{3\eta\lambda_2}{k}[4k\sin(2k)+(2-4k^2)\cos(2k)-2] + \frac{\eta\lambda_1}{2k^3}[(-2k^4+6k^2-3)\cos(2k) + (4k^3-6k)\sin(2k)+3]\Big\}, \quad (21)$$

where

$$\lambda_1=\frac{(1+2\eta)^2}{(1-\eta)^4}, \quad (22)$$

$$\lambda_2=-\frac{(1+\eta/2)^2}{(1-\eta)^4}, \quad (23)$$

and $\eta=4\pi\rho/3$ is the reduced density of the security spheres.

The integral (20) must then be numerically evaluated to finally obtain $S_2$ from (12) and (19). This was done by Torquato and Stell for systems of hard spheres in equilibrium, for which $\mu(r)=m(r)$. However, this is somewhat problematic for the current model of particles within security spheres, since in general $\mu(r)$ [and hence $\tilde{\mu}(k)$] may be either difficult or impossible to obtain analytically. Therefore, instead of using direct numerical integration to evaluate (20), we instead use a *one-dimensional* fast Fourier sine transform [25]. The function $\tilde{\mu}(k)$ may be obtained from the Fourier sine transform of $r\mu(r)$ by this method, as well as $M(r)$ from $k\tilde{M}(k)$.

In summary, for our model of impenetrable particles of random alignment within security spheres, the microstructure function $S_2(r)$ may be obtained from (12). The quantity $\mathcal{V}_2(r)$ is essentially a geometric function, while the double integral (19) may be numerically evaluated using the Fourier transform of $\mu(r)$ and the solution of the Ornstein-Zernike equation under the Percus-Yevick approximation.

### C. Simplification of $S_3$

We now consider the simplification of (7) for $n=3$. Once again, we follow the method of Torquato and Stell [12] and find that

$$\begin{aligned} S_3(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = 1-\rho\mathcal{V}_3(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)+\rho^2[X(1,2)+X(1,3) \\ +X(2,3)]-\rho^2[Y(1;2,3)+Y(2;1,3) \\ +Y(3;1,2)]-\rho^3 Z(1,2,3). \end{aligned} \tag{24}$$

This formula is obtained after eliminating all terms which integrate to zero because of the impenetrability of the security spheres. In this formula, $\mathcal{V}_3(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$ is the expected union volume of three aligned particles with centers at $\mathbf{x}_1$, $\mathbf{x}_2$ and $\mathbf{x}_3$, averaged over all possible (common) orientations. Also, the terms *X*, *Y* and *Z* are given by

$$X(i,j)=\int\int \mu(x_{i4})g(r_{45})\mu(x_{j5})d\mathbf{x}_4\, d\mathbf{x}_5, \tag{25}$$

$$Y(i;j,k)=\int\int \mu(x_{i4})\mu_2(\mathbf{x}_{j5},\mathbf{x}_{k5})g(r_{45})d\mathbf{x}_4\, d\mathbf{x}_5, \tag{26}$$

and

$$\begin{aligned} Z(i,j,k)=\int\int\int \mu(x_{i4})\mu(x_{j5})\mu(x_{k6}) \\ \times g_3(\mathbf{x}_4,\mathbf{x}_5,\mathbf{x}_6)d\mathbf{x}_4\, d\mathbf{x}_5\, d\mathbf{x}_6, \end{aligned} \tag{27}$$

where

$$g_3(\mathbf{x}_4,\mathbf{x}_5,\mathbf{x}_6)=\rho(\mathbf{x}_4,\mathbf{x}_5,\mathbf{x}_6)/\rho^3. \tag{28}$$

## III. EVALUATION OF $S_2$ FOR SPHERICAL CORES AND ELLIPSOIDS

In the previous section, we developed a general analytical expression for $S_n$ for our model of impenetrable and randomly aligned particles within security spheres. We then simplified this expression for $S_1$, $S_2$, and $S_3$. In this section, we consider the explicit numerical evaluation of $S_2$ for two different examples of this model: spherical cores and randomly aligned ellipsoids.

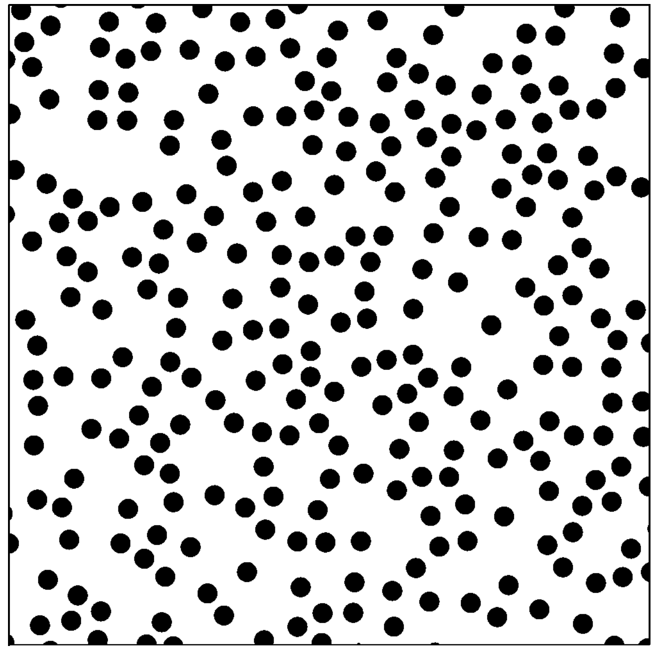

FIG. 2. A system of impenetrable disks with $\phi_2=0.175$. These particles are the cores of radius $\lambda=1/\sqrt{2}$ of a system of security spheres in equilibrium with volume fraction $\phi_2^s=0.35$. There is a positive minimal distance between the surfaces of any two particles.

### A. Spherical cores

The first specific model is really a deterministic model: we take the particles to be the cores of radius $\lambda<1$ within the security spheres. To illustrate this idea, a two-dimensional realization of this model with $\phi_2=0.175$ and $\lambda=1/\sqrt{2}$ (so that $\phi_2^s=0.35$) is shown in Fig. 2. This is not a simple model of impenetrable disks, since there is a *positive* minimal distance between the surfaces of two particles. For comparison, a system of disks in equilibrium with $\phi_2=0.175$ is shown in Fig. 3. In this figure, we see there are several particles which are almost touching.

For the model of three-dimensional spherical cores, the orientation of the cores is insignificant, and so the function $\mu$ is given by

$$\mu(r)=\begin{cases} 1, & r<\lambda, \\ 0, & r\geqslant\lambda. \end{cases} \tag{29}$$

The Fourier transform $\tilde{\mu}(k)$ may be analytically derived as

$$\tilde{\mu}(k)=\frac{4\pi}{k^3}[\sin(\lambda k)-\lambda k\,\cos(\lambda k)]. \tag{30}$$

Therefore, the double integral (19) may be obtained by either Fourier sine transforms, as above, or by direct numerical integration by using (21) and (30). We have used both methods as a check of our computer implementations, and we find that the two evaluations of $S_2$ are essentially the same.

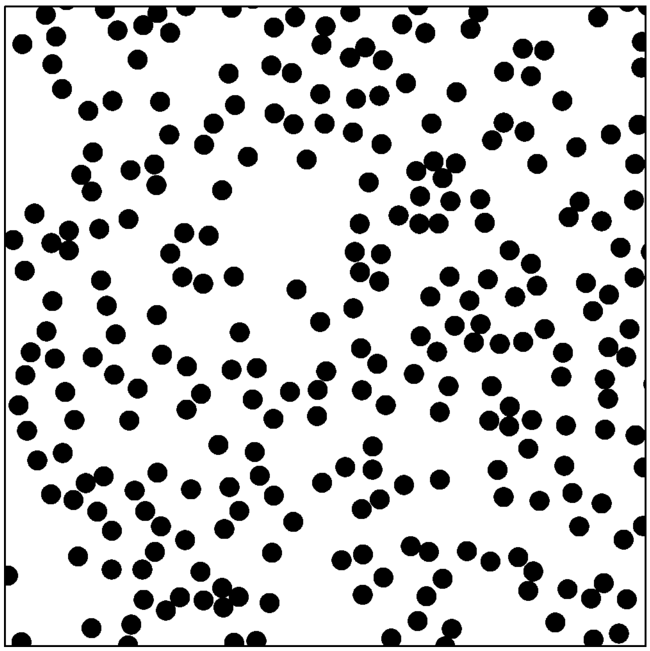

FIG. 3. A system of impenetrable disks in equilibrium with $\phi_2 = 0.175$.

In Fig. 4, we show the graphs of $S_2(u)$ for three systems of impenetrable cores. We show the dimensionless distance $u = r/\lambda$, normalized by the radius of the cores $\lambda$. We choose $\lambda$ to have the values 0.75, 0.85, and 1. (Of course, $\lambda = 1$ corresponds to ordinary impenetrable spheres.) To ensure that the volume fraction of the core phase is $\phi_2 = 0.2$ for each $\lambda$, the volume fraction of the security spheres is chosen to be

$$\phi_2^s = \phi_2 / \lambda^3. \tag{31}$$

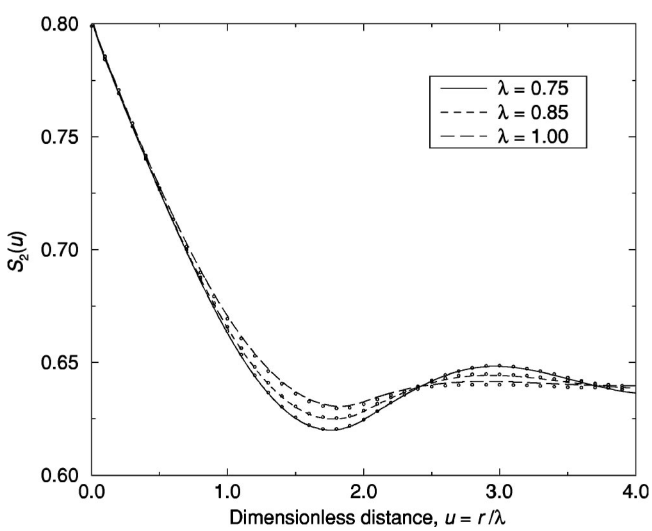


FIG. 4. The graphs of $S_2(u)$ for three systems of impenetrable cores. The volume fraction of the core phase is $\phi_2 = 0.2$, while the core radius $\lambda$ is chosen to be 0.75, 0.85, and 1. We see that the general shape of the function is the same for these different values of $\lambda$, but decreasing the size of the core heightens the crests and deepens the troughs. The circles are simulation data.

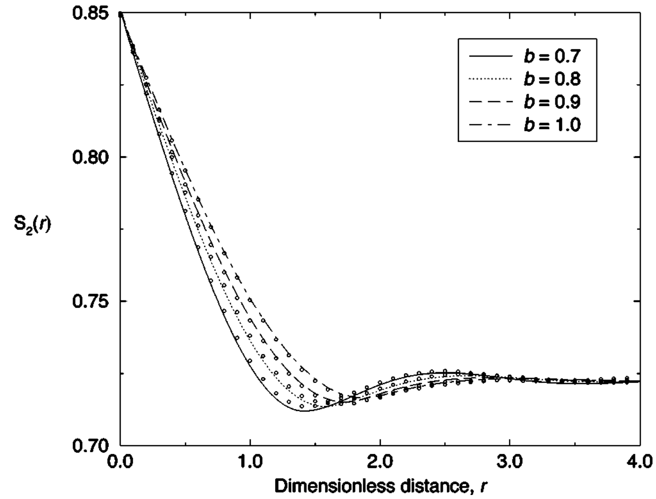


FIG. 5. The graphs of $S_2(r)$ for three systems of nonaligned ellipsoids. The volume fraction of the ellipsoids is $\phi_2 = 0.15$, while the common semiminor axes are chosen to have lengths $b = 0.70$, 0.80, 0.90, and 1. Naturally, $b = 1$ corresponds to a system of impenetrable spheres. The distance $r$ is measured in terms of the radius of the security spheres. We see that the first trough occurs for smaller $r$ as the ellipsoids become thinner and thinner. The circles are simulation data.

Of course, since $\phi_2^s < 1$ (not to mention the random close packing limit), the possible values of $\lambda$ for a given $\phi_2$ are constrained. The small circles are obtained from measuring $S_2$ from the cores of 1000 security spheres; the locations of the security spheres are determined by a molecular dynamics computer simulation. We see that the analytical and numerical calculations are in excellent agreement with simulations. We also see that the general shape of the graph of $S_2$ is unchanged by the choice of $\lambda$; however, smaller cores accentuate the crests and troughs.

### B. Randomly oriented oblate ellipsoids

We now consider particles which are oblate spheroids. In this model, the orientation of the individual particles is a

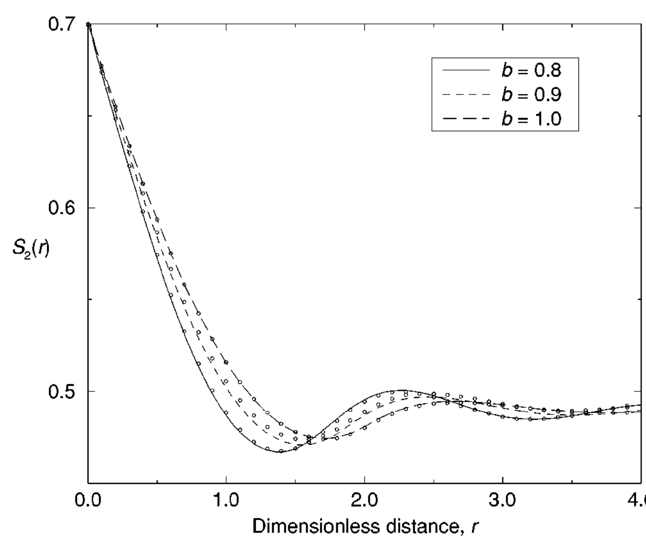


FIG. 6. As in Fig. 5, except with $\phi_2 = 0.3$ and $b = 0.80$, 0.90, and 1.

nontrivial complication (unlike the previous model of spherical cores.) The base particle has surface given by the equation

$$x^2+\frac{y^2}{b^2}+\frac{z^2}{b^2}=1,\quad b\leqslant 1, \tag{32}$$

so that the semimajor axis is equal to the radius of the security spheres. These ellipsoids share the same center as the security spheres but may be oriented at any angle. An illustration of this model in two dimensions was given in Fig. 1.

A simple calculation shows that the intersection volume of two *aligned* oblate ellipsoids, obtained by translating the center of the base ellipsoid to $\mathbf{x}_1$ and $\mathbf{x}_2$, is given by

$$V_2^{int}(\mathbf{x}_1,\mathbf{x}_2)=\begin{cases}\frac{4\pi}{3}b^2\left(1-\frac{3r_2}{4}+\frac{r_2^3}{16}\right), & r_2<2,\\ 0, & r_2\geqslant 2\end{cases} \tag{33}$$

where

$$r_2=\left(x_0^2+\frac{y_0^2}{b^2}+\frac{z_0^2}{b^2}\right)^{1/2} \tag{34}$$

and $\mathbf{x}_2-\mathbf{x}_1=(x_0,y_0,z_0)$.

To obtain $\mathcal{V}_2(r)$, we use the relation

$$\mathcal{V}_2(r)=2V_1-\mathcal{V}_2^{int}(r)=\frac{8\pi ab^2}{3}-\mathcal{V}_2^{int}(r), \tag{35}$$

where $\mathcal{V}_2^{int}(r)$ is the expected intersection volume of two aligned oblate ellipsoids, averaged over all possible orientations of the two particles. This is equivalent to averaging (33) over all vectors $(x_0,y_0,z_0)$ with length $r$. After converting to spherical coordinates, we find that

$$\mathcal{V}_2^{int}(r)=\frac{1}{4\pi}\int_{-\pi}^{\pi}\int_0^{2\pi}V_2^{int}(\theta,\phi)\sin\phi\, d\theta\, d\phi, \tag{36}$$

where

$$V_2^{int}(\theta,\phi)=\begin{cases}\frac{4\pi}{3}b^2\left(1-\frac{3r_2}{4}+\frac{r_2^3}{16}\right), & r_2<2,\\ 0, & r_2\geqslant 2,\end{cases} \tag{37}$$

and (34) simplifies to

$$r_2=\frac{r}{b}(1-[1-b^2]\cos^2\phi)^{1/2}. \tag{38}$$

After integrating, we finally obtain

$$\mathcal{V}_2^{int}(r)=\begin{cases}\frac{4\pi b^2}{3}\left[1+\frac{r(3r^2+2b^2r^2-48b^2)}{128b^2}-\frac{3r(16b^2-r^2)\arcsin(\sqrt{1-b^2})}{128b^3\sqrt{1-b^2}}\right], & 0\leqslant r\leqslant 2b,\\ 1-\frac{3r}{8}+\frac{r^3}{64}+\frac{3r^3}{128b^2}-3\left(\frac{r^2+8b^2}{64b^2}\right)\sqrt{\frac{r^2-4b^2}{r^2(1-b^2)}} \\ \quad+\frac{3r(r^2-16b^2)\left[\arcsin(\sqrt{1-b^2})-\arcsin\left(\sqrt{1-\frac{r^2}{4b^2}}\right)\right]}{128b^3\sqrt{1-b^2}}, & 2b\leqslant r\leqslant 2,\\ 0, & r>2.\end{cases} \tag{39}$$

To calculate $S_2(r)$ for this model using (12), we also need the function $\mu(r)$. Unlike the two examples above, this function is no longer deterministic since the particles are permitted to have different orientations within the security spheres. Since the ellipsoids are oblate, it is a straightforward calculus exercise to show that

$$\mu(r)=\begin{cases}1, & 0\leqslant r\leqslant b,\\ 1-\frac{1}{r}\sqrt{\frac{r^2-b^2}{1-b^2}}, & b\leqslant r\leqslant 1,\\ 0, & r\geqslant 1.\end{cases} \tag{40}$$

The functions (35), (39), and (40) are then substituted into (12) and (19) to numerically evaluate $S_2$.

In Figs. 5 and 6, we show the graphs of $S_2(r)$ for systems of impenetrable ellipsoids with $\phi_2=0.15$ and $\phi_2=0.3$, respectively. The dimensionless distance $r$ is proportional to the radius of the security spheres. Also, a range of values of $b$ are chosen; of course, setting $b=1$ changes the ellipsoids into spheres. For a system of impenetrable nonaligned ellipsoids, the volume fraction of the security spheres is given by

$$\phi_2^s=\phi_2/b^2. \tag{41}$$

The small circles again are obtained from computer simulations by measuring $S_2$ for systems of 1000 randomly aligned ellipsoids within security spheres. We see that the theoretical predictions are in excellent agreement with computer simulations. For small values of $b$, the peaks and troughs are accentuated and are shifted to somewhat smaller dimensionless distances. This shift makes intuitive sense: the length scale of the particles (and hence $S_2$) decreases with $b$.

## IV. CONCLUSIONS

We have introduced a model of random media consisting of particles, placed within security spheres, with arbitrary fixed shape and random orientation. We have developed a general expression for $S_n$ for this model and have simplified this expression for $S_1$, $S_2$, and $S_3$. Finally, we have numerically evaluated $S_2$ for spherical cores and randomly aligned ellipsoids. We have observed that the composition of the material is reflected in the graph of $S_2$.

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