Porosity for the penetrable-concentric-shell model of two-phase disordered media: Computer simulation results

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Computer-simulation results are reported for the porosity of a model of two-phase random media composed of identical D-dimensional spheres ($D = 2$ or 3) distributed with an arbitrary degree of impenetrability λ, $0 \leqslant \lambda \leqslant 1$; $\lambda = 0$ corresponding to randomly centered or "fully penetrable" particles and $\lambda = 1$ corresponding to totally impenetrable particles. We specifically consider the D-dimensional penetrable-concentric-shell model in which each sphere of diameter σ is composed of a mutually impenetrable core of diameter $\lambda\sigma$, encompassed by a perfectly penetrable concentric shell of thickness $(1-\lambda)\sigma/2$. We develop two independent techniques to sample for the porosity. Simulation results agree with known exact results for the extreme limits of $\lambda = 0$ and $\lambda = 1$ up to three significant figures. The results for intermediate λ are new and compare favorably with approximate analytical expressions obtained by Rikvold and Stell.

I. INTRODUCTION

The quantitative characterization of the microstructure of disordered two-phase media is a problem of great technological and fundamental interest in many fields, ranging from the physical to the biological sciences. Among the numerious applications are heat or electrical conduction in composite media,[1] diffusion of oxygen in tissues,[2] wave propagation in porous media,[3] fluid flow in porous media,[4] elastic response of particulate- and fiber-reinforced materials,[5] chromatography and filtration,[4,6,7] and chemical reactions in heterogeneous media.[8] The transport, mechanical, electromagnetic, and chemical properties of two-phase media, in general, depend upon an infinite set of statistical correlation functions which characterize the microstructure.[9–11] Since a complete statistical characterization of the microstructure is generally out of the question, one must rely upon the utilization of limited microstructural information, i.e., lower-order correlation functions. The simplest and most basic of these functions is the volume fraction of one of the phases, say phase 1, which we generally refer to (in the language of porous media) as the porosity ϕ_1. Determination of the porosity for a certain interpenetrable-particle model is the subject of the present work.

Many two-phase materials, such as packed beds, suspensions, and porous media, are characterized by "topological asymmetry" between the two phases. (In cases where the microstructure of phase 1 at volume fraction ϕ_1 is identical to that of phase 2 when the volume fraction of phase 1 is $1-\phi_1$, the composite is said to possess topological symmetry). Useful models of topologically asymmetric materials are random distributions of identical D-dimensional spheres (which can be considered to be fluid, solid, or void) of volume fraction $\phi_2 = 1 - \phi_1$ embedded in a host matrix of volume fraction or "porosity" ϕ_1. We specifically consider D-dimensional spheres (where $D = 2$ or 3) in the penetrable-concentric-shell (PCS)[12] model. In the PCS model (depicted in Fig. 1), each sphere (disk) of radius $\sigma/2$ is composed of an impenetrable core of radius $\lambda\sigma/2$, encompassed by a perfectly penetrable concentric shell of thickness $(1-\lambda)\sigma/2$. The extreme limits $\lambda = 0$ and 1 correspond, respectively, to the cases of fully penetrable (i.e., randomly centered) and totally impenetrable particles.

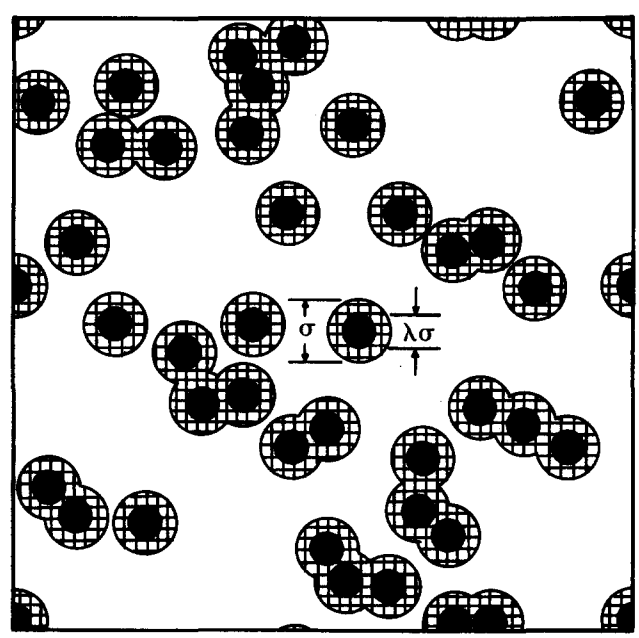

FIG. 1. A computer-generated realization of a distribution of disks of radius $\sigma/2$ (shaded region) in the PCS model. The disks have an hard core of diameter $\lambda\sigma$ indicated by the smaller, black circular region. Here $\lambda = 0.5$ and volume fraction of disks is approximately 0.3.

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The PCS model is versatile in that it enables one to vary the degree of the connectedness of the particle phase by varying the degree of impenetrability λ. For example, for 3D equilibrium ensembles of fully penetrable ($\lambda = 0$) and totally impenetrable ($\lambda = 1$) spheres, the particle phase percolates (i.e., a sample-spanning cluster appears) at a sphere volume fraction ϕ_2 of about 0.3 (Ref. 13) and 0.64 (Ref. 14), respectively. (A distribution of fully penetrable spheres is actually a bicontinuous medium for $0.3 \leqslant \phi_2 \leqslant 0.97$, where $\phi_2 = 0.97$ corresponds to the point at which the matrix phase fails to percolate.[15]) Thus, the PCS model can be employed to study both media with a discontinuous particle phase (e.g., suspensions) and materials possessing a continuous particle phase (e.g., polymer blends, sandstones, sintered materials, cermets, etc.). Recently, the PCS model and its variants have been studied in the context of continuum percolation.[16–18]

The central question addressed in this study is the following: Given the particle number density ρ and the degree of impenetrability λ, what is the porosity ϕ_1 (or the particle-phase volume fraction ϕ_2)? The volume fraction is clearly a more general and, thus, important statistical average than the number density since the former quantity remains well defined for systems in which there are no well-defined inclusions. For the extreme cases $\lambda = 0$ and 1, the porosity expressions are well known[9] and are, respectively, given by

$$\phi_1 = \exp(-\eta) \tag{1}$$

and

$$\phi_1 = 1 - \eta , \tag{2}$$

where $\eta = \rho V_1$ is a reduced number density (which for $\lambda = 0$ varies between 0 and ∞) and V_1 is the volume of a D-dimensional sphere (i.e., for $D = 1$, 2, and 3, $V_1 = \sigma$, $\pi\sigma^2/4$, and $\pi\sigma^3/6$, respectively). For intermediate λ and arbitrary η, the theoretical determination of the porosity is nontrivial. From a simulation standpoint, the problem also becomes nontrivial if the degree of overlap is nonzero, i.e., for $0 \leqslant \lambda < 1$.

For distribution of particles, Torquato and Stell[9] developed integral representations of the porosity (and its higher-order generalizations) in terms of the n-particle distribution functions ρ_n which characterize the probability of finding a particular configuration of n particles. In studying the effect of connectivity of the particle phase on the effective conductivity of a dispersion of spheres, Torquato[12] used the aforementioned formalism to obtain the low-density expansion of ϕ_1 in the PCS model for the arbitrary λ:[19]

$$\phi_1 = 1 - \eta + I_D(\lambda)\eta^2 + O(\eta^3) , \tag{3}$$

where I_D are D-dependent integrals[12] given by

$$I_2 = 2(1-\lambda^2) - \frac{1}{\pi}\left[\frac{3\pi}{2} + (1-4\lambda^2) \times \sin^{-1}\lambda - 3\lambda(1-\lambda^2)^{1/2} + 2\lambda(1-\lambda^2)^{3/2}\right], \tag{4}$$

$$I_3 = 4(1-\lambda^3) - \tfrac{9}{2}(1-\lambda^4) + (1-\lambda^6) . \tag{5}$$

The exact evaluation of successively higher-order terms in the Torquato–Stell[9] series representation of ϕ_1 becomes increasingly difficult and ultimately intractable because all of the ρ_n (quantities which, for $n \geqslant 2$, are at best known approximately analytically) are required to compute the multidimensional integrals involved. By establishing an isomorphism between the PCS model and scaled-particle theory, Rikvold and Stell[7] were able to obtain analytical expressions for the porosity for the PCS model in the scaled-particle approximation.

The purpose of this article is to compute, for the first time, the porosity ϕ_1 as a function of η and λ for D-dimensional spheres ($D = 2$ and 3) in the PCS model from Monte Carlo simulations.[20,21] Although the case $\lambda = 1$ is a trivial one to calculate, instances where $\lambda < 1$ are nontrivial to compute from simulations because of interparticle overlap. We develop two independent techniques to sample for ϕ_1 (or, equivalently, ϕ_2).

In Sec. II, we describe the simulation techniques we develop to determine the porosity for the D-dimensional PCS model from Monte Carlo simulations. In the subsequent section, we report our results for the porosity as a function of η and λ, and compare them to the scaled-particle approximations due to Rikvold and Stell.[7] Finally, in Sec. IV, we make some concluding remarks.

II. SIMULATION PROCEDURE

Obtaining statistical measures such as the porosity and related quantities[20,22,23] from computer simulations is a two-step process. First one must generate realizations of the random medium. Subsequently, one samples each realization for the desired quantity and then averages over a sufficiently large number of realizations. In what follows, we describe the details of our simulation methods to accurately obtain the porosity or, more precisely, the complementary particle-phase volume fraction $\phi_2 = 1 - \phi_1$ for equilibrium distributions of identical disks and spheres in the PCS model.

Consider each D-dimensional sphere to have a diameter σ and an inner impenetrable core of diameter $\lambda\sigma$. In order to generate equilibrium realizations for fixed λ and reduced number density η, we employed a conventional Metropolis algorithm.[24] Particles were initially placed, with no hard core overlaps, in a cubical cell of volume L^D [$(L/\sigma)^2 = 625$ and $(L/\sigma)^3 = 512$] on the sites of a regular array (square and body-centered-cubic arrays for $D = 2$ and 3, respectively). The cell was surrounded by periodic images of itself. Each particle was then moved (by some small amount) to some new position which was accepted or rejected according to whether or not the inner hard cores overlapped. This process was repeated many times until equilibrium was achieved. For $D = 2$, each of our simulation consisted of 10 400 moves per particle, the first 400 of which were discarded before sampling for equilibrium properties. The volume fraction was sampled at intervals of 100 moves per particle. In three dimensions, each simulation consisted of 2400 moves per particle, the first 400 of which were not included in the statistical averaging, with sampling occuring every 20 moves per particle. In order to ensure that equilibrium was achieved, we determined the pressure as a function of η for system of particles having diameter $\lambda\sigma$. The pressures ob-

tained were in very good agreement with accurate determinations of it made in previous studies.[25,26]

The volume fraction ϕ_2 is equivalent to the probability of finding a randomly thrown point in the particle phase. Therefore, a natural way to compute ϕ_2 is to throw many points randomly into the two-phase medium and record the ratio of the total number of successes to the total number of attempts. This procedure by itself turns out to be inefficient and inaccurate. For example, we found that throwing 5×10^5 points per realization was not enough to obtain statistically acceptable results: our goal being to measure ϕ_2 to within three significant figures. In light of this, we examined other schemes to sample for ϕ_2.

Each of our methods to measure ϕ_2 involves storing the positions of each particle in a configuration and a "digitized" image[20] of the configuration. A digitized image is obtained by dividing the system volume into square (cubical) pixels, e.g., in 2D we employed a resolution of 500×500 pixels. Initially all pixels in the pixel array are "unpainted" (an integer 0 is assigned to each pixel). If a pixel lies entirely in the particle phase it is painted (and integer 1 is assigned). If it contains an edge of the two-phase interface, the pixel is assigned a particle identification number which ranges from 2 to $N+1$, where N is the total number of particles. Pixels containing more than one particle edge are stored with their corresponding particle identification numbers on a separate table. Associated with each column of the table are the particle identification numbers and each pixel is denoted by the negative of the corresponding column number.

In principle, the volume fraction ϕ_2 is the sum of two contributions: the fraction of pixels which lie entirely in the particle phase (the number of integer 1's in the array) plus the fraction of particle phase in each pixel which contains the two-phase interface. Thus, the nontrivial part of the problem reduces to computing the latter contribution. In the 2D case, we developed two independent methods to determine the particle-phase volume fraction of the interface pixels. For the 3D problem, we used a procedure which is a slightly modified version of one of the two methods employed in the 2D instance. In all our simulations, the reduced denstiy η was varied by varying the number of particles while keeping the size of the particles fixed. This enabled us to keep the pixel resolution fixed for all η. The effect of system size on our results was studied. For the number of particles we employed, we found that our results (within statistical error) did not depend on the system size.

We now describe the details of the sampling procedure used in two and three dimensions.

A. Two dimensions

In 2D we developed two different techniques to measure the volume fractions of the pixels containing an edge of the two-phase interface: the random sampling method and a modified GRID method. In the random-sampling method, we randomly throw a number of points in each interface pixel and check to determine whether they fall within a disk. If $\mathbf{r}_i$ represents the position vector locating the center of particle i and $\mathbf{s}$ denotes the position of the random point, then the attempt is counted as a success if

$$|\mathbf{r}_i-\mathbf{s}|\leqslant\sigma/2 \quad \text{for any } i=1,2,3,\ldots,n\,, \tag{6}$$

where n is the number of particles whose surfaces pass through a given pixel. This way of sampling is somewhat similar to the "cell-list" method employed previously[22] to measure the two-point probability function of the matrix phase for totally impenetrable spheres. There are two key differences: (i) whereas in Ref. 22 the points were thrown over the entire system volume, here they were thrown in interface pixels only, and (ii) the cells in Ref. 22 contained at most one particle (having a volume of the order of the volume of a particle) and hence were much larger than the pixels used in the present study (which are approximately 310 and 270 pixels per particle in 2D and 3D, respectively).

In the random sampling method, we threw 50 points per interface pixel. This is equivalent to sampling as many as 1.25×10^7 points per realization if they were thrown over the entire system volume. In general, the system volume fraction was determined to within three significant figures using this method.

For our 2D simulations, we also employed a modified GRID[20] method. Here we assumed that each interface pixel had a particle-phase volume fraction of unity if the center of the pixel was contained in the particle phase or zero otherwise. This method is essentially the GRID[20] method where each particle is approximated by a collection of pixels whose centers are in the given particle. The GRID method was used to accurately determine the two-point matrix probability function.[22] The only modification made here is that the particle centers are not restricted to be located exactly at the nearest pixel center. Clearly, the error associated with the GRID method diminishes as the resolution increases. For the resolution used in our calculations, we found the modified GRID method to produce results as accurate or even more accurate than the random-sampling method. Henceforth, we refer to the modified GRID method as simply the GRID method.

B. Three dimensions

Both methods described above were tested to measure ϕ_2 in the 3D case. For 3D media, the number of interface pixels increases approximately by a factor of the number of pixels per diameter (in this case 20) relative to 2D case, and hence the random-sampling method requires an excessive amount of computing time. On the other hand, the GRID method requires an excessive amount of memory in order to use a sufficiently fine resolution. (Note that we use a 32 bit integer word per pixel.)

In order to overcome these difficulties, we use a two-step GRID method: (i) first we tesselated the system into larger pixels (a resolution of $64\times64\times64$ as opposed to $500\times500\times500$) and identified particle-phase, pore-phase, and interface pixels as aforementioned, (ii) then we tesselated further each interface pixel into 27 subpixels and assumed that each subpixel had a particle-phase volume fraction of unity if the center of the pixel was contained in the particle phase or zero otherwise. This is equivalent to the GRID method with the higher resolution of $192\times192\times192$ (i.e., 24 pixels per diameter). The results obtained using the two-

step GRID method were found to be even more accurate than the already accurate 2D results.

III. RESULTS AND DISCUSSION

We examined the volume fraction of the particle phase ϕ_2 in the PCS model in both two and three dimensions for various values of reduced number density η and impenetrability parameter λ using the computer-simulation methods described in the previous section. All simulations were carried out on an IBM 3090 and an IBM 4341. The CPU time spent for all calculations was, if converted to that of the IBM 3090, over 15 h for 2D and over 30 h for 3D (without vectorizing).

First we report results for the two extreme cases of fully penetrable particles ($\lambda = 0$) and totally impenetrable particles for which we have the exact results (1) and (2). In Tables I and II we report 2D results for $\lambda = 0$ and $\lambda = 1$, respectively. In each table we give the volume fraction as obtained from the random-sampling and GRID methods up to digits where the first difference appears between them. The statistical errors listed for each value of η were calculated from the mean square deviations for the ensemble of realizations. The statistical errors are small in general; however, the errors for $\lambda = 0$ are larger than for $\lambda = 1$. This is expected since the major source of statistical fluctuations is directly related to the degree of overlap $1 - \lambda$. For totally impenetrable particles ($\lambda = 1$), the actual volume fraction of the system remains constant from realization to realization and is known exactly *a priori* because of the simple relation of ϕ_2 to the total number of particles N. For penetrable particles, on the other hand, even though N remains fixed in the simulation, the actual volume fraction will fluctuate from realization to realization because of overlap. We also give the root mean square deviation δ between the simulation and exact values defined by

$$\delta = \left[\frac{1}{M} \sum_{i=1}^{M} \{ (\phi_{2,i}^{\mathrm{MC}} - \phi_{2,i}^{\mathrm{Exact}}) / \phi_{2,i}^{\mathrm{Exact}} \}^2 \right]^{1/2}, \tag{7}$$

where M is the total number of η values reported. Note that generally δ is small, with the GRID method being the more accurate of the two procedures. In summary, the 2D results for $\lambda = 0$ and 1 are accurate up to three significant figures.

In Table III we list analogous results for the 3D instance using the two-step GRID method. The statistical errors and the rms deviations from the exact results are, in general, even smaller then they are in the corresponding 2D problems.

TABLE I. Monte Carlo simulation data for the volume fraction of disks as a function of reduced density η for $\lambda = 0$ obtained by the GRID and random sampling methods. The statistical errors were calculated from the mean square deviations for the ensemble of realizations. $\delta = 0.000\,66$ and 0.001 12 for the GRID and random sampling methods, respectively. Here δ is the rms deviation from the exact values defined by Eq. (7) and $V_1 = \pi/4$.

η/V_1	GRID method	Random sampling	Exact
0.32	0.222 19 ± 0.003 48	0.222 84 ± 0.003 20	0.222 23
0.64	0.395 47 ± 0.005 85	0.394 94 ± 0.006 14	0.395 08
0.96	0.529 50 ± 0.006 26	0.529 18 ± 0.006 61	0.529 51
1.28	0.633 79 ± 0.007 11	0.634 27 ± 0.007 33	0.634 07
1.60	0.715 32 ± 0.007 42	0.715 42 ± 0.007 53	0.715 39
1.92	0.779 45 ± 0.007 60	0.778 91 ± 0.007 48	0.778 64
2.24	0.827 12 ± 0.007 01	0.828 45 ± 0.005 58	0.827 83

TABLE II. Monte Carlo simulation data for the volume fraction of disks as a function of reduced density η for $\lambda = 1$ obtained by the GRID and random sampling methods. The statistical errors were calculated from the mean square deviations for the ensemble of realizations. $\delta = 0.000\,62$ and 0.000 87 for the GRID and random sampling methods, respectively. Here δ is the rms deviation from the exact values defined by Eq. (7) and $V_1 = \pi/4$.

η/V_1	GRID method	Random sampling	Exact
0.08	0.062 87 ± 0.000 17	0.062 89 ± 0.000 14	0.062 83
0.16	0.125 74 ± 0.000 35	0.125 77 ± 0.000 31	0.125 66
0.24	0.188 62 ± 0.000 49	0.188 67 ± 0.000 39	0.188 50
0.32	0.251 48 ± 0.001 06	0.251 55 ± 0.001 13	0.251 33
0.48	0.377 2 ± 0.001 7	0.377 3 ± 0.001 8	0.376 99
0.64	0.503 0 ± 0.001 7	0.503 1 ± 0.001 5	0.502 65
0.80	0.628 7 ± 0.001 6	0.628 8 ± 0.001 5	0.628 32

We now describe our results for intermediate values of λ (i.e., $0 < \lambda < 1$): the range of λ for which there are no exact results. For the 2D case, we studied $\lambda = 0.3, 0.5, 0.7, 0.8$, and 0.9. In the 3D instance, we examined $\lambda = 0.5$, 0.7, 0.8, and 0.9. The values of η were restricted such that the hard-core volume $\eta\lambda^D$ did not exceed the rigid-particle phase transition point which is equal to approximately 0.69 and 0.49 in two and three dimensions, respectively (see Refs. 24–26 and references therein). The statistical errors range between 0.006 (for $\lambda = 0.3$) and 0.000 07 (for $\lambda = 0.9$) in 2D, and between 0.003 (for $\lambda = 0.5$) and 0.000 04 (for $\lambda = 0.9$) in 3D. In general, statistical errors were found to increase with decreasing λ for reasons mentioned earlier. Our raw data is summarized in Tables IV and V for 2D and 3D, respectively. Keeping in mind that the deviations of our simulation data for $\lambda = 0$ and 1 from the exact results [Eqs. (1) and (2)] are at least one order smaller than statistical errors (cf. Tables I–III) and assuming that the same accuracy is expected for all λ, we again claim that our results are accurate up to three significant figures.

As noted earlier, Rikvold[7] and Stell obtained analytical expressions for the porosity for the PCS model in the scaled-particle approximation. Their results are given as

$$\phi_1(\eta,\lambda) = (1 - \lambda^D \eta) \exp\left[- \frac{(1 - \lambda^D)\eta}{1 - \lambda^D \eta} \right] F_D(\eta,\lambda), \tag{8}$$

where

$$F_2(\eta,\lambda) = \exp\left[- \frac{\lambda^2 \eta^2}{(1 - \lambda^2 \eta)^2} (1 - \lambda)^2 \right] \tag{9}$$

in two dimensions, and

$$F_3(\eta,\lambda) = \exp\left\{ \frac{-3\lambda^3 \eta^2}{2(1 - \lambda^3 \eta)^3} \times [2 - 3\lambda + \lambda^3 - (3\lambda - 6\lambda^2 + 3\lambda^3)\lambda^3 \eta] \right\} \tag{10}$$

in three dimensions. In the extreme limits, $\lambda = 0$ and $\lambda = 1$, Eq. (8) gives exact results for all η [cf. Eqs. (1) and (2)]. For $0 < \lambda < 1$ in 2D, Eqs. (8) and (9) are exact through the

TABLE III. Monte Carlo simulation data for the volume fraction of spheres as a function of the reduced number density η for $\lambda = 0$ and 1 obtained using the two-step GRID method. Stastistical errors were calculated from mean square deviations for the ensemble of realizations. $\delta = 0.001\,06$ and $0.000\,01$ for $\lambda = 0$ and 1, respectively. Here δ is the rms deviation from the exact values and $V_1 = \pi/6$.

	$\lambda = 0$		$\lambda = 1$	
η/V_1	Simulation	Exact	Simulation	Exact
0.125	$0.063\,43 \pm 0.000\,75$	0.063 35	$0.065\,45 \pm 0.000\,04$	0.065 45
0.250	$0.122\,75 \pm 0.002\,08$	0.122 69	$0.130\,90 \pm 0.000\,06$	0.130 90
0.375	$0.177\,98 \pm 0.001\,99$	0.178 28	$0.196\,35 \pm 0.000\,09$	0.196 35
0.500	$0.230\,52 \pm 0.003\,22$	0.230 33	$0.261\,80 \pm 0.000\,21$	0.261 80
0.625	$0.279\,40 \pm 0.003\,03$	0.279 10	$0.327\,25 \pm 0.000\,00$	0.327 25
0.750	$0.324\,98 \pm 0.004\,10$	0.324 77	$0.392\,71 \pm 0.000\,25$	0.392 70
0.875	$0.367\,95 \pm 0.004\,40$	0.367 55	$0.458\,16 \pm 0.000\,37$	0.458 15

level of the second virial coefficient which implies that they are exact through first order in η [cf. Eqs. (3) and (4)], i.e., Eq. (8) for 2D becomes inexact in the second-order density term. This can be verified by comparing the density expansion of Eq. (8) [in conjunction with Eq. (9)] to Eqs. (3) and (4). In fact, one can show that Eq. (8) for 2D and $0 < \lambda < 1$, through second order in η, overestimates the true porosity or equivalently, underestimates the particle-phase volume fraction. On the other hand, for $0 < \lambda < 1$ in 3D, the scaled-particle approximation (8) is exact through the level of the third virial coefficient, i.e., it predicts a porosity which is exact through second order in η [cf. Eq. (3)].

Simulation results are compared with the scaled-particle approximations (8)–(10) in Figs. 2 and 3 for 2D and 3D, respectively. Plotted are the volume fractions of the included phase ϕ_2 as a function of the hard-core volume fraction $\eta\lambda^D$ for given values of λ. In general, the scaled-particle approximations are in good agreement with the simulation data; deviations from the data become more pronounced for λ intermediate between the two extreme limits $\lambda = 0$ and $\lambda = 1$, albeit small deviations. The agreement is better in 3D than in 2D which is consistent with the low-density discussion given above. Moreover, in 2D, simulation data are generally slightly above the scaled-particle predictions; this again is consistent with the fact that at low densities the 2D expression is a lower bound on ϕ_2. For the 3D case, simulation results are in general slightly below the scaled-particle results.

TABLE IV. Monte Carlo simulation data for the volume fraction of disks ϕ_2 as a function of the reduced number density η for various values λ. The statistical errors were calculated from mean square deviations for the ensemble of realizations and range between 0.006 and 0.000 07. Here $V_1 = \pi/4$.

η/V_1	$\lambda = 0.3$	$\lambda = 0.5$	$\lambda = 0.7$	$\lambda = 0.8$	$\lambda = 0.9$
0.08	···	···	0.062 58	0.062 75	0.062 80
0.16	···	0.1223	0.124 5	0.125 2	0.125 6
0.24	···	···	0.185 7	0.187 4	0.188 3
0.32	0.2293	0.2378	0.246 2	0.249 1	0.250 9
0.40	···	···	0.305 5	0.310 3	0.313 5
0.48	···	0.3459	0.364 1	0.371 3	0.375 8
0.56	···	···	0.177 4	0.431 2	0.438 0
0.64	0.4168	0.4461	0.477 2	0.490 5	0.499 9
0.72	···	···	0.531 4	0.548 7	0.561 3
0.80	···	0.5383	0.584 4	0.605 7	0.622 3
0.88	···	···	0.635 1	0.661 3	0.682 5
0.96	0.5684	0.6213	0.683 9	0.714 8	0.741 6
1.04	···	···	0.729 5	0.766 1	0.799 1
1.12	···	0.6953	0.773 6	0.814 2	···
1.20	···	···	0.813 6	0.859 3	···
1.28	0.6871	0.7609	0.850 8	0.899 3	···
1.36	···	···	0.884 0	0.934 2	···
1.44	···	0.8173	0.913 2	0.959 0	···
1.52	···	···	0.938 2	···	···
1.60	0.7792	0.8646	0.958 3	···	···
1.68	···	···	0.974 3	···	···
1.76	···	0.9029	···	···	···
1.92	0.8480	0.9339	···	···	···
2.24	0.8990	0.9737	···	···	···
2.56	0.9349	0.9925	···	···	···
2.88	···	0.9987	···	···	···
3.20	0.9764	···	···	···	···
4.48	0.9982	···	···	···	···

TABLE V. Monte Carlo simulation data for the volume fraction of spheres ϕ_2 as a function of the reduced number density η for various values of λ. The statistical errors were calculated from mean square deviations for the ensemble of realizations and range between 0.003 and 0.000 04. Here $V_1 = \pi/6$.

η/V_1	$\lambda = 0.5$	$\lambda = 0.7$	$\lambda = 0.8$	$\lambda = 0.9$
0.125	···	···	···	0.065 446
0.250	0.126 21	0.129 256	0.130 30	0.130 83
0.375	···	···	···	0.1961 13
0.500	0.243 29	0.254 52	0.258 81	0.261 33
0.625	···	···	···	0.326 33
0.750	0.350 94	0.374 42	0.384 58	0.391 11
0.875	···	···	···	0.455 56
1.000	0.448 34	0.488 06	0.506 33	0.519 55
1.125	···	···	···	0.582 94
1.250	···	0.593 50	0.622 18	0.646 10
1.500	0.615 79	0.689 47	0.726 37	···
1.750	···	0.774 03	0.824 75	···
2.000	0.746 63	0.845 69	···	···
2.250	···	0.902 95	···	···
2.500	0.843 155	0.950 60	···	···
2.750	···	0.980 05	···	···

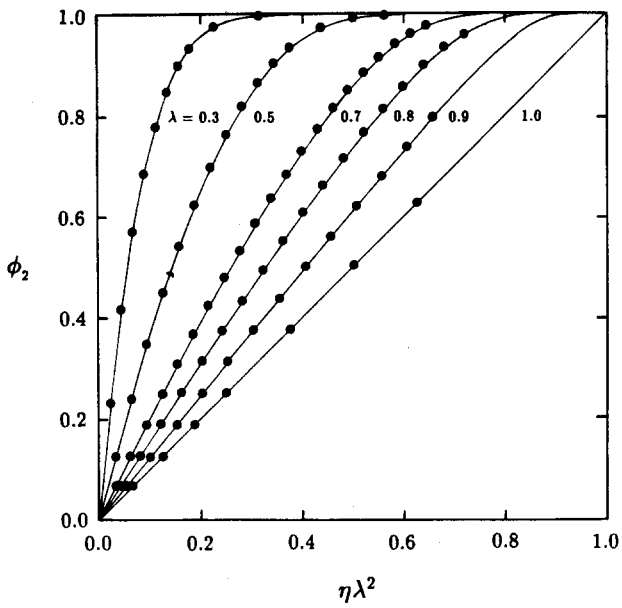

FIG. 2. Volume fraction of disks ϕ_2 versus hard-core volume fraction $\eta\lambda^2$ for given values of the impenetrability parameter λ. Points are our computer-simulation results. Solid lines are obtained from the scaled-particle approximation (8) for the porosity $\phi_1 = 1 - \phi_2$.

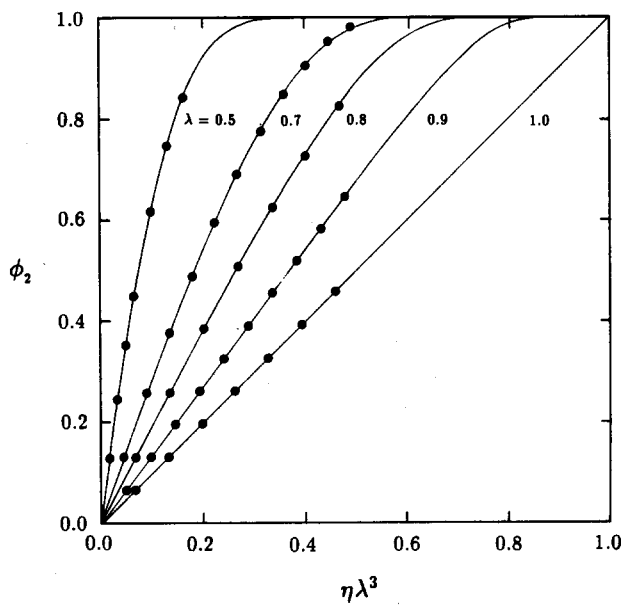

FIG. 3. Volume fraction of spheres ϕ_2 versus hard-core volume fraction $\eta\lambda^3$ for given values of the impenetrability parameter λ. Points are our computer-simulation results. Solid lines are obtained from the scaled-particle approximation (8) for the porosity $\phi_1 = 1 - \phi_2$.

IV. CONCLUSIONS

We have devised accurate methods to obtain the porosity or the particle-phase volume fraction for the PCS model of two-phase random media from Monte Carlo simulations. The most accurate procedure is the two-step GRID method. It is believed that the two-step GRID method can be applied to accurately ascertain the porosity for general models of two-phase random media as well. Finally, we have determined that the Rikvold–Stell scaled-particle approximations for the porosity in the PCS model provide good estimates of it.

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