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Spatial correlations in polydisperse, frictionless, two-dimensional packings

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We investigate next-nearest-neighbor correlations of the contact number in simulations of polydisperse, frictionless packings in two dimensions. We find that disks with few contacting neighbors are predominantly in contact with disks that have many neighbors and vice versa at all packing fractions. This counterintuitive result can be explained by drawing a direct analogy to the Aboav-Weaire law in cellular structures. We find an empirical one parameter relation similar to the Aboav-Weaire law that satisfies an exact sum rule constraint. Surprisingly, there are no correlations in the radii between neighboring particles, despite correlations between contact number and radius.

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Disordered packings of particles are the quintessential model for amorphous materials such as granular packings [1], emulsions [2], wet foams [3], and glass formers [4]. While the contact number distribution and its average near the random close-packing density [1–3,5–9] have been extensively studied in these systems, little is known about spatial correlations in the contact network. Various models that have recently been put forward to predict the density [10], distribution of contact numbers [2], and forces [11] in random close packings implicitly assume the absence of such correlations.

We address this question through simulations of a two-dimensional model system with polydisperse, frictionless soft disks. At the random close-packing density ϕ_c, the disks just touch and have an average contact number $\langle z\rangle$ close to 4 as required for mechanical stability [1,12,13]. Due to disorder the individual contact numbers z are distributed according to some distribution $P(z)$ that depends on the polydispersity of the disk size distribution [2]. Here, we investigate whether spatial correlations in the contact network exist.

In our simulations we find that disks with many contacts favor neighbors with fewer contacts and vice versa. These correlations persist for all packing densities. This result is a direct analog to the well-known Aboav-Weaire law in the field of cellular structures which states that cells with fewer neighbors are surrounded by cells with many neighbors [14–18]. We show that our results are in excellent agreement with a modified Aboav-Weaire law. Since geometrical constraints in the packing dictate that smaller particles have fewer contacts on average [2], one may expect similar correlations for the size distribution in the packing, namely, that larger particles are surrounded by smaller ones. Surprisingly, we find that the size of the central particle is uncorrelated to the average size of the contacting neighboring particles.

We simulate the disordered packings by using Durian's soft disk model [9], as implemented by Langlois *et al.* [19]. The disks have a harmonic repulsion proportional to their overlap and experience viscous tangential drag. We use 1500 polydisperse disks whose radii are drawn from a Gaussian distribution with a mean $\langle r\rangle$ and a variance $\sigma_2 = (0.304\langle r\rangle)^2$. The polydispersity allows us to access a wide range of contact numbers, which is important to measure next-nearest-neighbor correlations. The disks are randomly placed in a periodic box at low packing fraction and then allowed to relax while their radii are slowly increased. The simulation terminates when the total elastic energy due to overlaps reaches a steady state at a predefined packing fraction. For each packing density, up to 10 different packings are created to increase the statistics of our correlation measures. Upon reaching mechanical equilibrium, disks with fewer than three contacts (rattlers) are removed for the analysis of the contact network but are accounted for in the packing fraction. Contacts are defined as overlaps between disks.

We study packings which range from the random close packing density ϕ_c up to $\phi = 1.35$. Note that the overlap area between bubbles is counted twice in the calculation of ϕ in line with previous simulations of packings [1]. In our simulations we find $\phi_c = 0.845$ and the corresponding average contact number $\langle z\rangle = 4.07 \pm 0.04$, which is close to the isostatic prediction $\langle z\rangle = 4$ [1]. As shown in the inset of Fig. 1, $\langle z\rangle$ increases approximately as $4 + 3.29\sqrt{\phi - \phi_c}$, close to the isostatic point, which is consistent with previous results [6,7]. We study packings up to $\phi = 1.35$, where the average contact number reaches $\langle z\rangle = 6$.

Figures 1(a) and 1(b) show the distribution of the relative contact number, $P(z - \langle z\rangle)$, for different packing fractions and their respective variance $\mu_2 = \langle z^2\rangle - \langle z\rangle^2$, where $\langle z^i\rangle = \sum_z z^i P(z)$. The shape of the distribution is independent of the packing fraction as evidenced by the collapse of $P(z - \langle z\rangle)$ onto a master curve. The corresponding variance μ_2 varies slightly due to the fact that the minimum contact number is 3. This collapse is surprising and means that the the shape of $P(z)$ around its mean depends on $P(r)$ but not on ϕ.

Next, we address the main result of our work—the correlations in the contact network of the packings at different densities. Given a disordered packing of frictionless disks with a certain global average contact number $\langle z\rangle$, are the *local* contact numbers of neighboring particles correlated? Here, we define neighbors to be disks in contact, i.e., disks that overlap. In order to quantify nearest-neighbor correlations, we measure $m(z)$, which is the average contact number of the neighbors of a disk with contact number z.

This approach is analogous to the pioneering work of Aboav [17] on polycrystals, which established spatial correlations in the coordination number of cells in a cellular structure. He found that many-sided cells are surrounded by few-sided cells on average and vice versa. It has been noted by Weaire

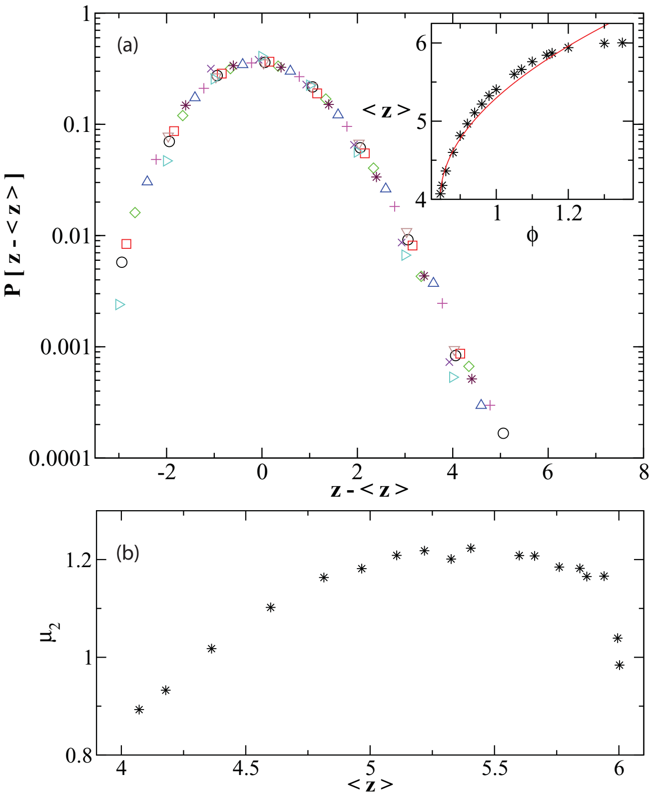

FIG. 1. (Color online) (a) The contact number distribution $P(z - \langle z\rangle)$ for different packing fractions ϕ: ($\times$) 0.845, ($*$) 0.88, ($\triangledown$) 0.92, (+) 0.96, ($\triangle$) 1.0, ($\Diamond$) 1.07, ($\Box$) 1.14, ($\bigcirc$) 1.2, and ($\triangleright$) 1.35. The inset shows the variation of the average contact number $\langle z\rangle$ with packing fraction ϕ. The red (solid) line corresponds to the square root scaling fit: $\langle z\rangle = 4 + z_0\sqrt{\phi - \phi_c}$, where $z_0 = 3.29$. (b) The variance of $P(z)$, μ_2, versus $\langle z\rangle$.

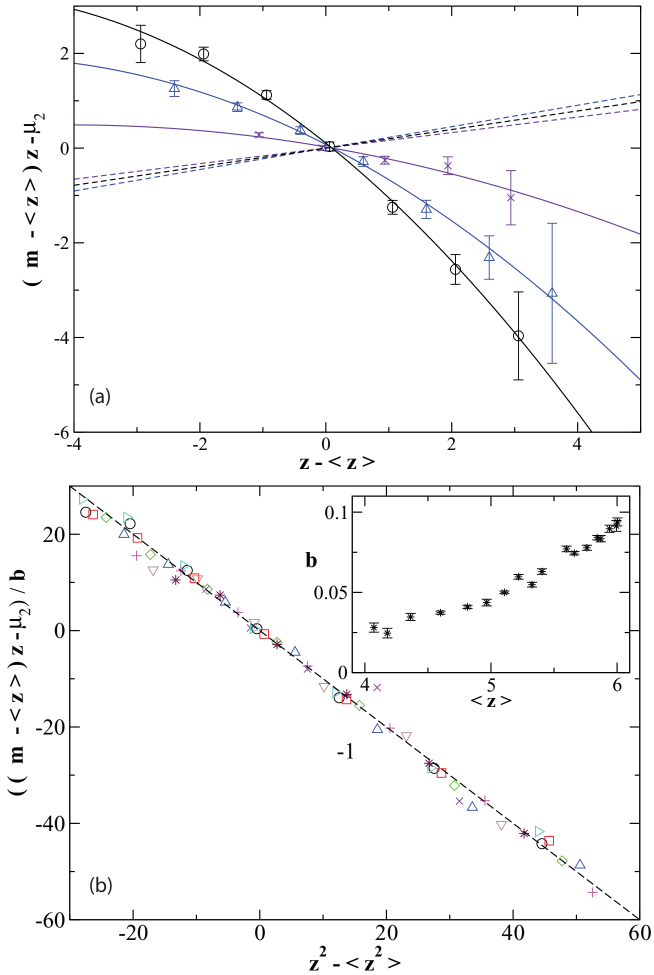

FIG. 2. (Color online) Nearest-neighbor correlations of the contact number. (a) $(m - \langle z\rangle)z - \mu_2$ versus $(z - \langle z\rangle)$ for three different densities: ($\times$) 0.854, ($\triangle$) 1.0, and ($\bigcirc$) 1.2. The error bars are standard deviations from the mean. The lines are fits to Eq. (4). The dotted lines correspond to the uncorrelated prediction $a = -\mu_2/\langle z\rangle$. (b) $[(m - \langle z\rangle)z - \mu_2]/b$ versus $(z^2 - \langle z^2\rangle)$ for all densities [same symbols as in Fig. 1(a)]. The dotted line corresponds to the slope -1. The inset shows the fit parameter b as a function of $\langle z\rangle$.

[18], that m obeys an exact sum rule which is independent of dimensionality:

$$\sum_z mzP(z) = \sum_z z^2 P(z), \quad (1)$$

where z is the coordination number of the cells. This sum rule is based on a counting argument and is independent of the physics governing the underlying structure. In the absence of correlations in the coordination number between neighboring cells, $m(z)$ is simply a constant ($\equiv \overline{m}$). It follows from the sum rule that in this case $\overline{m} = \langle z\rangle + \mu_2/\langle z\rangle$ [14]. In the context of cellular structures, this is referred to as a topological gas, although its existence is disputed [15]. The Aboav-Weaire relation is a solution of the sum rule

$$m = \langle z\rangle - a + (\langle z\rangle a + \mu_2)/z, \quad (2)$$

where a is an empirical parameter. For a topological gas, $a = -\mu_2/\langle z\rangle$, but in a natural cellular structure such as dry foam $a \approx 1$ [14,16]. Therefore, many-sided cells have few-sided neighbors and vice versa. One can interpret this anticorrelation as a partial screening of the topological charge $(z - \langle z\rangle)$ by its nearest neighbors whose combined charge is $z(m - \langle z\rangle)$. Even though the validity of Eq. (2) cannot be deduced from first principles, most two-dimensional (2D) cellular structures, such as polycrystals and dry foams, obey this relation well [15–17], with the notable exception of random Voronoi tessellations [20].

The counting argument that leads to the sum rule [Eq. (1)] was originally developed for cellular structures but holds equally well for neighbors in a contact network of a disordered packing. The main difference is that in 2D cellular structures with threefold vertices, $\langle z\rangle = 6$ [14], while frictionless packings in two dimensions have an average contact number $\langle z\rangle$ greater than or equal to 4 depending on the packing fraction [1,6].

The results for m are shown in Fig. 2(a), where we plot $(m - \langle z\rangle)z - \mu_2$ versus $(z - \langle z\rangle)$ for three different packing fractions. For the Aboav-Weaire law [Eq. (2)] to hold we expect the data to follow a line with slope $-a$. Clearly, the data do not follow the uncorrelated prediction $a = -\mu_2/\langle z\rangle$, instead we observe spatial correlations: disks with few contacts are surrounded by disks with many contacts and vice versa.

Another key result is the deviations from purely linear behavior, especially at higher packing fractions.

In order to account for this nonlinearity, we expand the Aboav-Weaire law in terms of the moments of the contact number distribution such that it still satisfies the sum rule

$$(m - \langle z\rangle)z - \mu_2 = -\sum_{i=1}^{\infty} c_i(z^i - \langle z^i\rangle), \qquad (3)$$

where the c_i's are arbitrary constants. If $c_i = 0$ for $i > 1$, one recovers the usual Aboav-Weaire law with $c_1 = a$. In order to fit our data it proved sufficient to only make c_2 nonzero, which leads to

$$m = \langle z\rangle - bz + \frac{\mu_2(1+b) + b\langle z\rangle^2}{z}, \qquad (4)$$

where $b = c_2$. This is a one parameter fit, similar to the Aboav-Weaire law. However, mz is now quadratic in z, instead of linear. As shown in Fig. 2(b), Eq. (4) captures the nonlinearity well and leads to a much improved fit compared to Eq. (2). Including higher-order terms in the expansion [Eq. (3)] does not improve the fit significantly. The inset of Fig. 2(b) shows the decrease of the parameter b with $\langle z\rangle$, which means that the screening of topological charge decreases as the isostatic point is approached.

We would like to stress that the analogy between correlations in the coordination number in disordered frictionless packings and cellular structures is not obvious, since these systems are governed by different local and global constraints. Although polydisperse packings can be tesselated into a cellular structure [2], not all faces of a cell correspond to contacts; therefore the existence of correlations in packings does not follow naturally from similar correlations in disordered cellular structures.

There is also a correlation between contact number and particle size in polydisperse packings [2]. Larger particles have more contacts on average, since one may fit more particles around them on average. Figure 3 shows the average contact number of a particle with radius r, $\langle z|r\rangle = \sum_z zP(z|r)$, where $P(z|r)$ is the conditional probability of a particle of radius r to have a contact number z. It is well described by the linear relation

$$\langle z|r\rangle = \langle z\rangle[1 + \gamma(r/\langle r\rangle - 1)]. \qquad (5)$$

Since $\langle z|r\rangle$ is constrained by the equality $\int_0^\infty \langle z|r\rangle P(r)dr = \langle z\rangle$, there is only one empirical fit parameter γ, which varies little with ϕ (Fig. 3, inset). However, this linear relationship does break down at low r, since $\langle z|r\rangle \geqslant 3$. A similar result exists in the field of cellular structures and is known as Lewis' law [15,21].

Given the nearest-neighbor correlations in the coordination number [Eq. (4)] and the correlation between size and contact number [Eq. (5)], are smaller particles surrounded by larger ones, similar to observations in cellular structures [22]?

In order to study radii correlations, we measured $\langle R_{nn}|r\rangle$, which is the average radius of neighboring disks in contact with a disk of radius r. Figure 4 shows $\langle R_{nn}|r\rangle/\langle r\rangle$ versus $r/\langle r\rangle$ for ϕ_c. No correlations are apparent and the result agrees well with the uncorrelated prediction $\overline{R_{nn}}$ which is discussed below.

The counting argument that leads to the Weaire sum rule for the coordination number can also be applied for the radii.

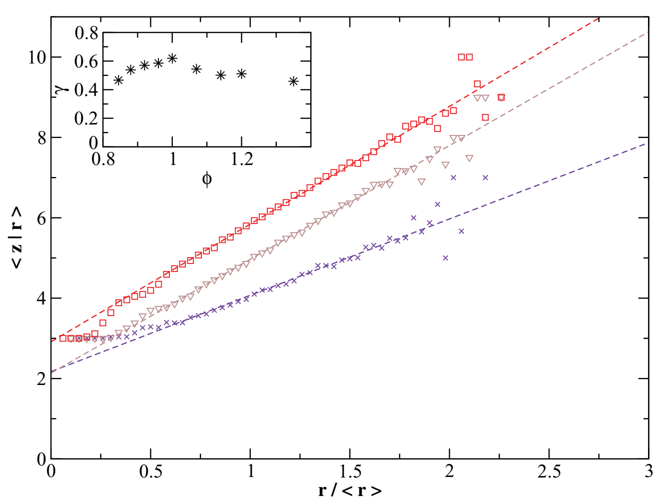

FIG. 3. (Color online) The average contact number $\langle z|r\rangle$ for a given particle radius r at different packing fractions ϕ: (×) 0.845, (▽) 0.92, and (□) 1.14. Lines are fits to Eq. (5). The inset shows the fit parameter γ as a function of ϕ.

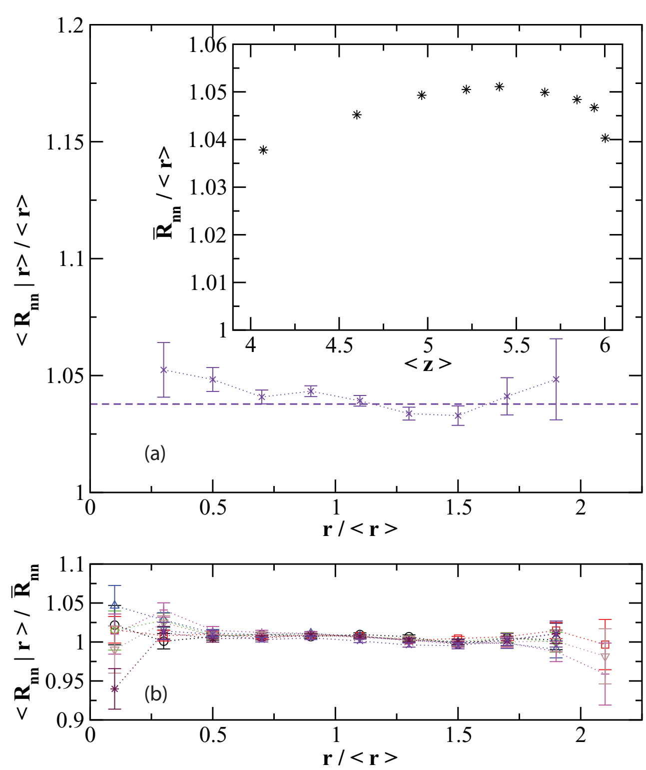

FIG. 4. (Color online) Nearest-neighbor correlations of the radii. (a) $\langle R_{nn}|r\rangle$ versus $r/\langle r\rangle$ for $\phi = 0.845$. The dotted line corresponds to the uncorrelated prediction $\overline{R_{nn}}$ [Eq. (7)]. The inset shows $\overline{R_{nn}}$ versus $\langle z\rangle$. (b) $\langle R_{nn}|r\rangle/\overline{R_{nn}}$ versus $r/\langle r\rangle$ for all densities [same symbols as in Fig. 1(a)].

Analogously, the average radius of the neighbors $\langle R_{nn}|r\rangle$ needs to satisfy the following relation:

$$\int_0^\infty \langle R_{nn}|r\rangle\langle z|r\rangle P(r)dr = \int_0^\infty r\langle z|r\rangle P(r)dr \quad (6)$$

The left-hand side of the equation amounts to an integral over the disk radii r weighted by $\langle z|r\rangle$. In the absence of correlations $\langle R_{nn}|r\rangle$ is a constant ($\equiv \overline{R_{nn}}$), and we have

$$\overline{R_{nn}} = \frac{\int_0^\infty r\langle z|r\rangle P(r)dr}{\int_0^\infty \langle z|r\rangle P(r)dr} = \frac{\int_0^\infty r\langle z|r\rangle P(r)dr}{\langle z\rangle}. \quad (7)$$

Substituting the empirical relation for $\langle z|r\rangle$ [Eq. (5)], we find that $\overline{R_{nn}} = \langle r\rangle(1+\gamma\sigma_2/\langle r\rangle^2)$, which is slightly larger than $\langle r\rangle$ and varies little with ϕ [inset Fig. 4(a)]. At ϕ_c, we obtain $\overline{R_{nn}} = 1.042\langle r\rangle$, which is consistent with our results from Fig. 4(a). At higher packing fractions shown in Fig. 4(b), $\langle R_{nn}|r\rangle/\overline{R_{nn}}$ remains constant and close to 1. Only for high and low r are slight deviations due to low statistics observed.

While the absence of correlations in the radii for neighboring particles may be expected given our preparation procedure where particles are placed in the box at random, it is surprising in the light of the two correlations we have measured, namely, the correlations between contact numbers of neighboring particles [Eq. (4)] and the correlation between size and contact number [Eq. (5)]. The reason for this counterintuitive result is that the relationship between the average contact number m and the corresponding average radius R_{nn} does not follow the linear relation [Eq. (5)] for a single disk [23].

Although we have only shown results for packings with Gaussian distributed radii, similar correlations are observed for other polydispersities such as bidisperse distributions [23].

In conclusion, we studied polydisperse, frictionless packings at various packing densities. We find that disks with many contacts are surrounded by disks with few contacts and vice versa. As the isostatic point is approached, the screening of topological charges becomes weaker but does not vanish and is well described by a modified Aboav-Weaire law. This result is a direct analog of the topological screening observed in cellular structures. Nevertheless, the physical origin of the screening parameter b remains unclear, much like the a parameter in the Aboav-Weaire law [14].

We want to emphasize that the sum rules for the contact number and radii are valid in any dimension. Therefore, one may expect similar correlations in three-dimensional packings as well as in frictional packings [24]. It remains to be seen whether these correlations depend on the preparation history of the packing, which is known to have an influence on ϕ_c [25].

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