Local contact numbers in two dimensional packings of frictional disks

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We analyze the local structure of two dimensional packings of frictional disks numerically. We focus on the fractions \( x_i \) of particles that are in contact with \( i \) neighbors, and systematically vary the confining pressure \( p \) and friction coefficient \( \mu \). We find that for all \( \mu \), the fractions \( x_i \) exhibit powerlaw scaling with \( p \), which allows us to obtain an accurate estimate for \( x_i \) at zero pressure. We uncover how these zero pressure fractions \( x_i \) vary with \( \mu \), and introduce a simple model that captures most of this variation. We also probe the correlations between the contact numbers of neighboring particles.

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While soft frictionless spheres experience a critical jamming transition in the limit of zero pressure, where properties such as elastic moduli, contact number, density, characteristic frequencies and lengthscales exhibit powerlaw scaling [1, 2, 3, 4], the situation is more delicate for frictional systems. The approach to the jamming transition is still governed by the pressure, \( p \), but a range of densities and packing properties can exist depending on the value of the friction coefficient \( \mu \), the mobilization (ratio of frictional to normal forces) of the frictional contacts and the packing history [8]. In particular, in \( d \) dimensions, the contact number at jamming, \( z_c \), can take on a range of values between \( d+1 \) and \( 2d \), in contrast to frictionless sphere packings which always reach their respective isostatic contact number \( z_{iso}^0 = 2d \) at jamming. The proximity to the isostatic contact number governs the scaling near jamming — for frictionless spheres, properties such as elastic moduli scale with distance to jamming. However, for frictional packings these properties only scale with distance to the isostatic limit \( z_i^0 = d+1 \), and in general not with distance to jamming [1, 6, 7], although this depends on whether fully mobilized contacts are treated as frictional or slipping [8].

We recently studied the case of frictional spherical disks in two dimensions, and focussed on packings that were equilibrated very gently [6, 7, 8]. This eliminates preparation history and mobilization as unknowns: for given pressure \( p \) and friction coefficient \( \mu \), packings with well defined statistics are obtained. The gentle equilibration procedure also allows to approach the isostatic limit for frictional systems, \( z_c = z_{iso}^0 = d+1 \) when \( \mu \to \infty \) and \( p \to 0 \) — here jamming has many of the critical features observed for frictionless systems [6, 7].

One additional surprise is that for finite values of \( \mu \), such gently equilibrated packings still reach a generalized isostatic limit [5, 8]. This means, in short, that a substantial number of contacts get fully mobilized, i.e., their frictional forces \( f \) satisfy the bound \( |f_i| \leq f_n \), where \( f_n \) denotes the normal force. If these fully mobilized contacts are seen as slipping, the critical nature of the vibrational density of states at jamming is restored for all values of \( \mu \) [8].

Here we probe the fractions \( x_i(p=0,\mu) \) of particles with \( i = 2,3,\ldots,6 \) contact neighbors as function of the friction coefficient \( \mu \). The full curves are predictions from a simple model (Eqs. 1) with fixed variance \( \sigma^2 = 0.6 \).

FIG. 1: Variation of the fractions \( x_i(p=0,\mu) \) of particles with \( i = 2,3,\ldots,6 \) contact neighbors as function of the friction coefficient \( \mu \). The full curves are predictions from a simple model (Eqs. 1) with fixed variance \( \sigma^2 = 0.6 \).

Packings — Following [4], the numerical systems under consideration are two dimensional packings of 1000
spheres with 20% polydispersity in the diameter of the particles in a square box with periodic boundary conditions. The grains interact through 3D Hertz-Mindlin forces, i.e. with the normal force $f_{ij}$ between particles $i$ and $j$ proportional to $\delta_{ij}^{1/2}$, with $\delta_{ij}$ the overlap of the two particles. The Young modulus of the grains is set to 0.2, which determines the pressure unit, and the Poisson ratio is set to zero, while the unit of length is the average grain diameter. The construction and equilibration of the packings has been described in detail elsewhere [8, 9]. Rattlers, particles which have no appreciable interactions with any of the other particles, are always left out of the analysis of the packings and contact statistics. For each value of $\mu \in [10^{-3}, 10^3]$ and $p \in (10^{-6}, 10^{-3})$, 30 configurations were generated independently.

Scaling of fractions $x_i$ with pressure — As is shown in Fig. 2-a-c, $x_i(p, \mu)$ scales linearly with $p^{1/3}$, which allows us to extrapolate their values for finite $p$ to the (un)jamming limit at $p = 0$. This scaling is the same as the scaling of the total contact number $z$ with $p$, which for the Hertzian interactions employed here is consistent with the scaling that the excess contact number $\Delta z := z - z_c$ scales with the square-root of the excess packing fraction. This relation is well known for frictionless systems [1, 10], but also appears to hold for frictional systems [8, 11] — our data here suggests that it also holds for the individual contact fractions, irrespective of the value of $\mu$.

A second robust finding is illustrated in Fig. 2: the number of particles that have an odd number of contacts [12], is close to $1/2$ — the number of particles with an even or odd number of contacts is therefore approximately equal, irrespective of pressure or value of $\mu$. We do not have a satisfactory explanation for this.

The extrapolated fractions $x_i$ at jamming — In the remainder of this paper we focus on $x_i(\mu)$ at zero pressure. Since $x_i$ has to be zero for $i = 1$, and the fraction of particles with 7 contacts are negligible for the polydispersities employed here we focus on $i$ ranging from 2 to 6.

As shown in Fig. 3, the variation of $x_i$ with $\mu$ is greatest for $\mu$ between 0.1 and 1, with the small and large $\mu$ limits apparently well behaved.

The functional forms of $x_i(\mu)$ for $i = 3$ and 5 are similar, as are the functional forms of $x_i(\mu)$ for $i = 2$ and 4. This is related to the observations that $x_3 + x_5 \approx 1/2$. One also notices that, approximately, $x_2(\mu \to 0) \approx x_{n+1}(\mu \to \infty)$. In fact, for small $\mu$, the fractions $x_3$ and $x_5$ tend to 1/4, while $x_4$ approaches 1/2 for large $\mu$, $x_2$ and $x_4$ tend to 1/4, while $x_3$ approaches 1/2.

In the limits $\mu = 0$ or $\mu = \infty$, we can estimate these fractions by a very simple argument. Let us first focus on the zero friction case. Assuming that there are only particles with three, four or five contacts, the fractions $x_3$, $x_4$ and $x_5$ can immediately be calculated, since combining the condition that $x_3 + x_4 + x_5 = 1$ with the isostaticity condition $3x_3 + 4x_4 + 5x_5 = 4$ implies $x_3 = x_3$, and hence $x_3 = 1/4$, $x_4 = 1/2$ and $x_5 = 1/4$. A similar argument holds for $x_2$, $x_3$ and $x_4$ in the limit of infinite friction. Deviations from this result arise since a small fraction of particles with respectively six and five contacts arise, weakly breaking the “three particle species” condition underlying this argument (see Fig. 1).

Simple rate equation model — The ratios $x_3/x_4 = x_5/x_4 = 1/2$ can also be understood in terms of a simple stochastic model where we imagine distorting a certain packing, creating and breaking contacts but keeping the overall contact number and the ratios $x_i$ constant. In the case of three species only, particles with 4 contacts can become 3’s and 5’s, while 3’s and 5’s can only become 4’s (See Fig. 3). Since the transition probabilities must all be equal (since always two particles take place in such an event), and, on average, we require the fractions $x_i$ to be constant, we get, in this simple approximation,
$x_4 = 2x_3 = 2x_5$. This heuristic argument can be written as a rate equation model, as shown in Figure 4. Once we normalize the rates such that the total decay rate of each species is $2\omega$, we obtain as steady state $x_4 = 2x_3 = 2x_5$.

For intermediate values of $\mu$, the number of species is four (if we neglect a small number of $z = 6$-contacts). A single decay rate would than imply that $x_2 = 1/6$, $x_3 = 1/3$, $x_4 = 1/3$, $x_5 = 1/6$ and $z = 3.5$ — clearly a single rate does not capture the data. Figure 3 shows an extended model where we now associate an individual rate $\omega_i$ to each species $i$, so that the total decay rate of that species is $2\omega_i$. The solution to this model is $x_i \sim 1/\omega_i$ for $i = 3, 4$ and $x_1 \sim 1/(2\omega_1)$ for $i = 2, 5$.

Explicit solutions of rate equation model — We now seek an explicit solution of the four species model for the contact fractions as a function of the friction coefficient. To achieve this, we introduce two constraints on the model beyond the trivial normalization constraints $\sum_{i=2}^5 x_i = 1$ and $\sum_{i=j}^5 i x_i = z(\mu)$. First, we constrain our model by the empirical observation that the number of particles with odd and even contacts is equal, i.e., $x_3 + x_5 = 0.5$. Additionally, we impose the variance of the contact fraction distribution, $\sum_{i=2}^5 x_i(z - i)^2 = \sigma^2$. The solution to the resulting set of equations is

$$
x_2 = (\frac{(z - 4)^2}{4} - \sigma^2 + 1/2)/4
\text{ }x_3 = (\frac{-z - 3)^2 - \sigma^2 + 5/2}{4}
\text{ }x_4 = (\frac{-z - 4)^2 - \sigma^2 + 5/2}{4}
\text{ }x_5 = (\frac{(z - 3)^2 + \sigma^2 - 1/2}{4}
$$

To obtain definite predictions from this set of equations, we need to determine the variance $\sigma^2$. In the extreme limits, and under the simplifying assumption that only three species with fractions $1/4, 1/2, 1/4$ arise, we find $\sigma^2 = 0.5$ (notice if more species are present, $\sigma^2$ will be larger). Fixing now $\sigma^2 = 0.5$ over the whole range of friction coefficient, we obtain the prediction shown in figure 4. There are no additional fit parameters to this solution, and the agreement is quite good.

We have numerically studied the actual variance of $\sigma^2$ from the data, and find that for our data it varies between $0.57$ and $0.65$ — when we fix $\sigma^2 = 0.6$, the fit becomes significantly improved, as shown in Fig. 1.

Correlations — The rate equation model derives from its implicit assumption that the contact numbers of particles and their neighbors are uncorrelated. Based on this assumption, we can calculate the theoretical fraction $q_{ij}^{th}$ of contacts between particles with $i$ and $j$, given $x_i$ and $x_j$. Since the total fraction of contacts for particles with $i$ contacts is given by $ix_i/z$, the uncorrelated prediction for $q_{ij}$ is

$$
q_{ij}^{th} = \frac{2ix_i x_j}{z^2} \text{ for } i \neq j; \quad q_{ij}^{th} = \frac{ix_i x_j}{z^2} \text{ for } i = j
$$

Figure 3a shows the ratio $q_{ij}/q_{ij}^{th}$ of the observed fraction of contacts and the uncorrelated prediction [3]. For intermediate values of $i$ and $j$ the prediction is quite reasonable, as $q_{ij}/q_{ij}^{th}$ remains bounded between 0.5 and 1.6 or so. Contact pairs with very dissimilar $i$ and $j$ are favored - this is likely an effect of polydispersity, since small particles with few contacts prefer to sit next to larger particles with more contacts. A detailed study of this is left for the future.

In Figure 3b we have divided out the ratio at an intermediate $\mu$, to more clearly see the variation of $q_{ij}$ with $\mu$. This shows that the fractions corresponding to particles with $x_i$ that are abundant (such as $q_{44}$ for small $\mu$ and $q_{33}$ for large $\mu$) do not vary strongly with $\mu$. There appears to be a correlation between the relative over representation of contacts and the overabundance of the species of particles (i.e., for large $\mu$, there are many particles with 2 or 3 contacts, and $q_{33}$ is over abundant, while there are very few particles with 4 and 5 contacts, and the ratios $q_{44}$, $q_{45}$ and $q_{55}$ are even less likely) — we have no clear explanation for this.

Outlook — Simple arguments allow us to estimate the contact fractions $x_i$, which can be seen as fingerprints of the system. Since frictional systems depend on history, we expect the fractions and their variation to be a useful step in identifying the effects of preparation history beyond average values such as overall contact number and density.

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FIG. 5: (a) Ratio of the observed contact pair fraction $q_{ij}$ to the prediction $q_{ij}^{th}$ from equation 2 for all contact pairs with sufficient statistics. Contact pairs with very dissimilar $i$ and $j$ are favored. (b) Ratio of the observed contact pair fraction $q_{ij}$ to the prediction $q_{ij}^{th}$, rescaled by the ratio at $\mu = 0.32$. Contact pairs with large mean contact number reduce in frequency as $z$ drops, while pairs with small mean contact number show an upward trend.

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[12] Note that we approximate the number of particles with an odd number of contacts as $x_3 + x_5$. This is a good approximation as there are no particles with one contact, and very few with seven or more — for the largest pressures, $x_7 = 2.5 \times 10^{-3}$, and $x_7$ rapidly approaches zero for smaller pressures.
[13] Notice that we use here the values at the lowest pressure — extrapolating all these joint fractions for zero pressure leads to quite large error bars, since some joint fractions are very small.