Local contact numbers in two dimensional packings of frictional disks

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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 μ. We find that for all μ, the fractions x_i exhibit power-law 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 μ, and introduce a simple model that captures most of this variation. We also probe the correlations between the contact numbers of neighboring particles.

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 length-scales exhibit power-law scaling,[1–5] 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 μ, the mobilization (ratio of frictional to normal forces) of the frictional contacts and the packing history.[6–10] 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 $z_{iso}{}^{\mu} = d + 1$, and in general *not* with distance to jamming,[5–7] 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.[6–8] This eliminates preparation history and mobilization as unknowns: for given pressure p and friction coefficient μ, packings with well defined statistics are obtained. The gentle equilibration procedure also allows us to approach the isostatic limit for frictional systems, $z_c = z_{iso}{}^{\mu} = d + 1$ 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 μ, such gently equilibrated packings still reach a *generalized* isostatic limit.[7,8] The mobilization $m = |f_t|/\mu f_n$ of the contacts becomes an important variable, and in particular we find that a substantial number of contacts get fully mobilized, *i.e.*, their frictional forces f_t satisfy the bound $|f_t| \leq \mu f_n$, where f_n denotes the normal force. Such contacts cannot resist tangential perturbations, and hence they contribute only $d - 1$ constraints per contact to mechanical stability instead of d. Then the isostatic bound is changed to $z \geq (d + 1) + 2n_m/d$, where n_m is the mean number of fully mobilized contacts per particle. 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 μ.[8]

Here we probe the fractions $x_i(p)$ of particles that have i contacts for these frictional packings. These fractions are the simplest characteristics of the contact network beyond the average contact number z. It is thus natural to ask how the fractions x_i depend on p and μ. We find that, for given μ, the fractions $x_i(p)$ exhibit scaling with p similar to the scaling of the total contact number z. This allows us to extrapolate these fractions to $p \to 0$, and this is the case on which we focus our attention. As is shown in Fig. 1, the fractions x_i vary substantially with μ, and reach well-defined values in the limits where $\mu \to 0$ or $\mu \to \infty$. We find a number of simple but unexpected relations between the various x_i, and introduce a simple model that, given $z(\mu)$, gives a good prediction for $x_i(\mu)$.

Packings

Following ref. 11, the numerical systems under consideration are two dimensional packings of 1000 spheres with 20%

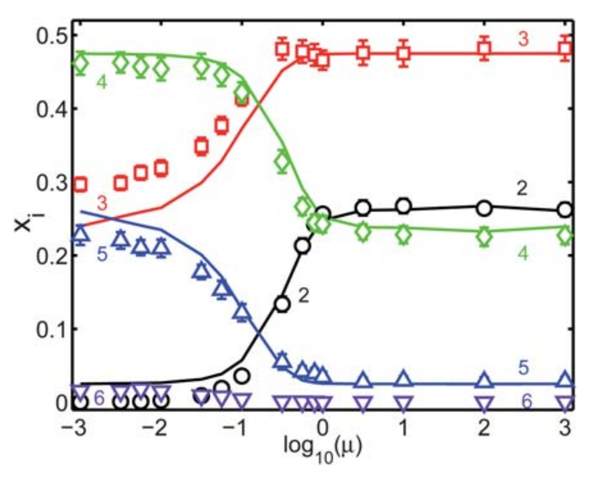

Fig. 1 Variation of the fractions $x_i(p = 0, \mu)$ of particles with $i = 2, 3, \ldots, 6$ contact neighbors as function of the friction coefficient μ. The full curves are predictions from a simple model (eqn (1)) with fixed variance $\sigma^2 = 0.6$.

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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 $\delta_{ij}^{3/2}$, with δ_{ij} the overlap of the two particles. The Young modulus of the grains is set to 1, 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 have been described in detail elsewhere.[7,11] 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. 2a–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,[1,12] but also appears to hold for frictional systems[6,13]—our data here suggests that it also holds for the individual contact fractions, irrespective of the value of μ.

A second robust finding is illustrated in Fig. 2d: the number of particles that have an odd number of contacts,[14] 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 μ. 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 is negligible for the polydispersities employed here we focus on i ranging from 2 to 6. As shown in Fig. 1, the variation of x_i with μ is greatest for μ between 0.1 and 1, with the small and large μ 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 observation that $x_3 + x_5 \approx 1/2$. One also notices that, approximately, $x_n(\mu \to 0) \approx x_{n+1}(\mu \to \infty)$. In fact, for small μ, the fractions x_3 and x_5 tend to 1/4, while x_4 approaches 1/2—for large μ, 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 $x_3 = x_5$, 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 Fig. 3a. Once we normalize the rates such that the *total* decay rate of each species is 2ω, we obtain as steady state $x_4 = 2x_3 = 2x_5$.

For intermediate values of μ, the number of species is four (if we neglect a small number of $z = 6$ contacts). A single decay rate would than imply that $\{x_2 \approx 1/6, x_3 \approx 1/3, x_4 \approx 1/3, x_5 \approx 1/6\}$ and $z = 3.5$—clearly a single rate does not capture the data. Fig. 3c shows an extended model where we now associate an individual rate ω_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 $x_i \sim 1/(2\omega_i)$ for $i = 2$, 5.

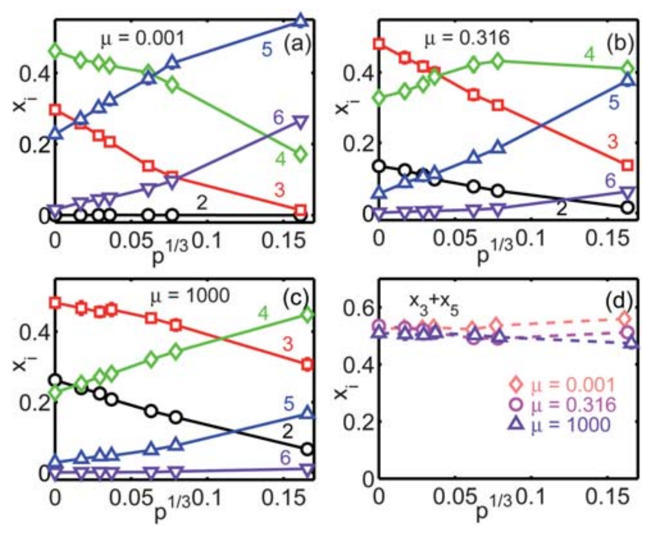

Fig. 2 Contact fractions x_i as a function of pressure. (a–c) For three representative values of μ, the x_i scale linearly with $p^{1/3}$ (equivalent to $\phi^{1/2}$ for the Hertzian interaction), and we are able to extrapolate to $p = 0$. (d) The sum $x_3 + x_5 \approx 0.5$, for all values of μ and p studied.

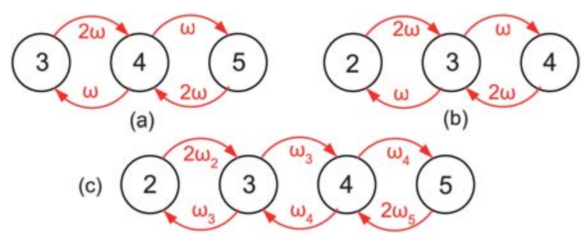

Fig. 3 Rate equation models for the equilibrium contact fractions. (a, b) A model with a single rate ω is sufficient for $\mu \to 0$ and $\mu \to \infty$. (c) For finite μ, we introduce individual rates ω_i which correspond to the total decay rate for contact number i.

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 $\sum_{i=2}^{5} i x_i = z(\mu)$. 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

$$
\begin{aligned}
x_2 &= \left((z-4)^2 + \sigma^2 - 1/2\right)/4 \\
x_3 &= \left(-(z-3)^2 - \sigma^2 + 5/2\right)/4 \\
x_4 &= \left(-(z-4)^2 - \sigma^2 + 5/2\right)/4 \\
x_5 &= \left((z-3)^2 + \sigma^2 - 1/2\right)/4
\end{aligned} \tag{1}
$$

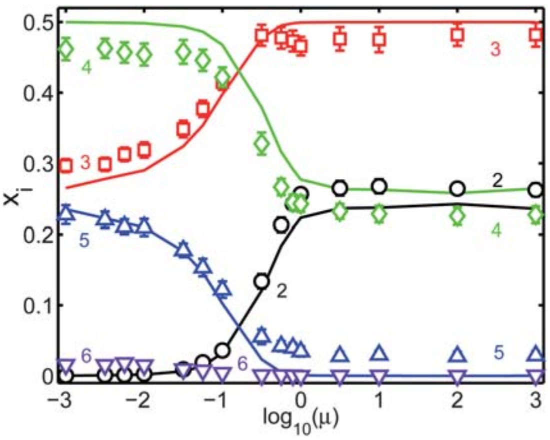

Fig. 4 Contact fractions as a function of μ in the extrapolated limit $p \to 0$. The curves show the model solution from eqn (1), with a variance $\sigma^2 = 0.5$.

To obtain definite predictions from this set of equations, we need to determine the variance σ^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 $\sigma^2 = 0.5$. We can show that for two species, $\sigma^2 = 0.5$ is a lower bound. For three species, it is possible to have a lower σ^2, for example close to $x_3 = x_5 = 0$, $x_4 = 1$. However, at the equilibrium point of the rate equation model, $x_2 = 1/4$, $x_4 = 1/2$, $x_5 = 1/4$, $\sigma^2 = 0.5$, while in the vicinity of this point, σ^2 is larger. When more species are introduced (as is the case for stronger polydispersity or in higher dimensions), we expect σ^2 to rise as well for the vast majority of packings. Note that for $d = 3$, the limiting contact numbers are $z = 4$ for infinite friction and $z = 6$ for vanishing friction, and hence the range of species will be different. There may be interesting exceptions for large size ratios; however, we do not expect to describe appolonian packings here. If we fix $\sigma^2 = 0.5$ over the whole range of friction coefficients, we obtain the prediction shown in Fig. 4. There are no additional fit parameters to this solution, and the agreement is quite good. We have numerically studied the actual variance of σ^2 from the data, and find that for our data, which have 20% polydispersity, 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

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

Fig. 5a shows the ratio q_{ij}/q_{ij}^{th} of the observed fraction of contacts and the uncorrelated prediction.[15] For intermediate values of i and j the prediction is quite reasonable, as q_{ij}/q_{ij}^{th}

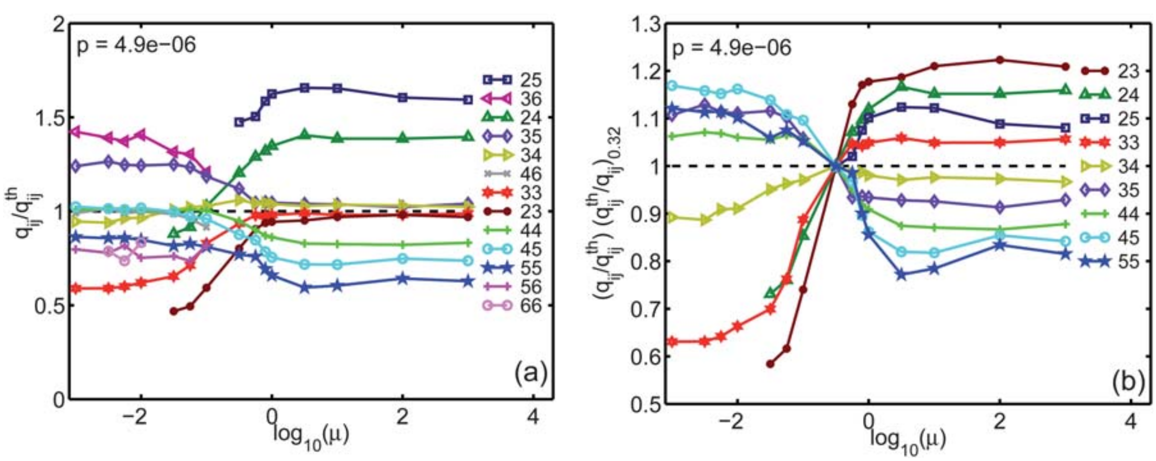

Fig. 5 (a) Ratio of the observed contact pair fraction q_{ij} to the prediction q_{ij}^{th} from eqn (2) for all contact pairs with sufficient statistics. The curves are labeled by the i and j of the pair. Contact pairs with very dissimilar i and j are favored. (b) Ratio of the observed contact pair 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.

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 Fig. 5b we have divided out the ratio at an intermediate μ, to more clearly see the variation of q_{ij} with μ. This shows that the fractions corresponding to particles with x_i that are abundant (such as q_{44} for small μ and q_{33} for large μ) do not vary strongly with μ. There appears to be a correlation between the relative over-representation of contacts and the over-abundance of the species of particles (*i.e.*, for large μ, there are many particles with 2 or 3 contacts, and q_{23} 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

Various studies concerned with predicting the local packing geometry have appeared recently.[9,16–19] Here we focus directly on the contact fractions for frictional packings, through probing which contact fractions are invariant under rearrangements. 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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14 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.
15 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.
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