Statistics of Frictional Families

Tianqi Shen,[1] Stefanos Papanikolaou,[2,1] Corey S. O'Hern,[2,1,3] and Mark D. Shattuck[4,2]
[1]Department of Physics, Yale University, New Haven, Connecticut 06520-8120, USA
[2]Department of Mechanical Engineering & Materials Science, Yale University, New Haven, Connecticut 06520-8260, USA
[3]Department of Applied Physics, Yale University, New Haven, Connecticut 06520-8120, USA
[4]Benjamin Levich Institute and Physics Department, The City College of the City University of New York, New York, New York 10031, USA

(Received 3 February 2014; published 15 September 2014)

We develop a theoretical description for mechanically stable frictional packings in terms of the difference between the total number of contacts required for isostatic packings of frictionless disks and the number of contacts in frictional packings, $m = N_c^0 - N_c$. The saddle order m represents the number of unconstrained degrees of freedom that a static packing would possess if friction were removed. Using a novel numerical method that allows us to enumerate disk packings for each m, we show that the probability to obtain a packing with saddle order m at a given static friction coefficient μ, $P_m(\mu)$, can be expressed as a power series in μ. Using this form for $P_m(\mu)$, we quantitatively describe the dependence of the average contact number on the friction coefficient for static disk packings obtained from direct simulations of the Cundall-Strack model for all μ and N.

DOI: 10.1103/PhysRevLett.113.128302 PACS numbers: 83.80.Fg, 45.70.-n, 81.05.Rm

Granular media are fascinating, complex materials that display gas-, liquid-, and solidlike behavior depending on the boundary and driving conditions. Frictional forces are crucial for determining the structural and mechanical properties of granular media in the solidlike state [1]. For example, friction plays an important role in setting the angle of repose [2], determining the width of shear bands in response to applied stress [3,4], and enabling arches to form and jam hopper flows [5].

For packings of frictionless spherical particles, it is well known that the minimum contact number required for mechanical stability [6] is $\langle z \rangle_{\min}^0 = 2N_c^0/N$, where $N_c^0 = dN - d + 1$ is number of contacts among N particles in the force-bearing backbone of the system (with periodic boundary conditions) and d is the spatial dimension. However, at a nonzero static friction coefficient μ, fewer contacts are required for mechanical stability with $N_c \geq N(d+1)/2 - 1 + 1/d$ and $\langle z \rangle_{\min}^\infty = d + 1$ in the large-N and -μ limits.

Several computational studies have measured the contact number as a function of μ for packings of frictional disks and spheres using "fast" compression algorithms that generate amorphous configurations [7–9]. In particular, these studies find $\langle z \rangle = \langle z \rangle_{\min}^0 = 4$ and $\langle z \rangle_{\min}^\infty = 3$ in the $\mu \to 0$ and ∞ limits, respectively, for bidisperse disks [10,11]. For intermediate values of μ, $\langle z \rangle$ smoothly varies between $\langle z \rangle_{\min}^0$ and $\langle z \rangle_{\min}^\infty$. However, it is not currently known what determines the contact number distribution for each μ and form of $\langle z(\mu) \rangle$ for a given packing preparation protocol. The ability to predict the functional form of the contact number with μ is important because $\langle z \rangle$ controls the mechanical [12] and vibrational [13] properties of granular packings.

In this Letter, we develop a theoretical description for packings of frictional disks at jamming onset in terms of their "saddle order," or the number of contacts that are missing relative to the isostatic value in the zero-friction limit, $m = N_c^0 - N_c$. In contrast, previous studies used $\mu \to \infty$ packings as the reference [14]. Using a novel numerical procedure (the "spring network" method) that allows us to enumerate packings for each m and molecular dynamics (MD) simulations of the Cundall-Strack model [15] for frictional disks, we show that m characterizes the dimension of configuration space that the packings occupy. Frictional packings with one missing contact ($m = 1$) form one-dimensional lines in configuration space, packings with $m = 2$ populate two-dimensional areas in configuration space, and packings with larger m form correspondingly higher-dimensional structures in configuration space. We assume that the probability for obtaining a packing with saddle order m at a given μ, $P_m(\mu)$, is proportional to the volume $V_m(\mu)$ occupied by force- and torque-balanced mth order saddle packings in configuration space. We find that $P_m(\mu)$ can be written as a power series in μ, $P_m(\mu) \sim a_m \mu^m / (1 + \sum_{m=1}^{m_{\max}} a_m \mu^m)$, where a_m are the normalized coefficients of the power series and $m_{\max}$ is the maximum number of contacts that can be removed in the $\mu \to \infty$ limit. Using this form, we quantitatively describe the dependence of the average contact number on the friction coefficient for disk packings obtained from MD simulations of the Cundall-Strack model over a wide range of μ and in the large system limit.

We generated packings of bidisperse (50:50 mixtures of particles with equal mass and diameter ratio $\sigma_1/\sigma_2 = 1.4$) frictional disks in square cells with periodic boundary conditions using two methods. First, we implemented a packing-generation algorithm in which the system is isotropically compressed or decompressed (followed by energy minimization) to jamming onset [6] at a packing fraction ϕ_J^m that depends on the saddle order. Pairs of overlapping disks i and j interact via repulsive linear spring forces $\vec{F}_{ij}^n$ in the direction of the center-to-center separation vector $\vec{r}_{ij}$. We implemented the Cundall-Strack model for the frictional interactions. When disks i and j come into contact, a tangential spring is initiated with a force $\vec{F}_{ij}^t$ that is proportional to the tangential (perpendicular to $\hat{r}_{ij}$) displacement u_{ij}^t between disks. u_{ij}^t is truncated so that the Coulomb threshold, $|\vec{F}_{ij}^t| \leq \mu|\vec{F}_{ij}^n|$, is always satisfied. When the disk pairs come out of contact, we set u_{ij}^t to zero.

The packings are distinguished in configuration space by plotting the second invariant $q_2 = [\mathrm{tr}^2(D) - \mathrm{tr}(D^2)]/2$ of the $N \times N$ distance matrix, $D_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$, versus ϕ_J^m (Fig. 1), where x_i and y_i are the x and y coordinates of particles i and j. (Note that q_2 is invariant to uniform translations and rotations, as well as particle-label permutations, of the system.)

We also developed a novel numerical technique (spring network method) to enumerate packings at each m. The method is best explained using an example. In Fig. 2(a), we show an $m = 0$ packing of $N = 6$ frictionless disks with $N_c = N_c^0 = 11$ contacts, which occurs in the lower right corner of the q_2-ϕ_J^m plane in Fig. 1(a). To generate $m = 1$ packings with ten contacts, we break one of the 11 contacts in this packing [e.g., the contact between disks 1 and 2 in Fig. 2(a)] and constrain its separation to be $r_{12}/\sigma_{12} = \lambda > 1$, while the other contacts are constrained to be $r_{ij} = \sigma_{ij}$. With these constraints and as a function of λ, we implement the successive compression and decompression packing-generation algorithm [6] to find packings at jamming onset, ϕ_J^1. This procedure is repeated for each of the ten other contacts in the packing in Fig. 2(a) to yield the $N_c^0 = 11$, $m = 1$ branches in Fig. 1(b), and then for each of the $m = 0$ packings. As shown in Fig. 1(b), we find overlap between the $m = 1$ branches from the spring network method and $m = 1$ packings generated from simulations of the Cundall-Strack model. $m = 2$ and higher-order saddle packings are obtained using a similar procedure, except multiple contacts are broken, as shown in Fig. 1(c). Thus, a collection of related packings with $N_b(N, m)$ branches originates with each $m = 0$ packing.

The plot of q_2 versus ϕ_J^m in Fig. 1(a) for packings with $m = 0$ and 1 illustrates several important features. First, in the $\mu \to 0$ limit, $m = 0$ packings occur as distinct points in configuration space (or q_2 versus ϕ_J^m) [6]. Second, as μ increases, $m = 1$ packings form one-dimensional lines in configuration space that emanate from $m = 0$ packings. The $m = 1$ packings that are stabilized at low μ are displaced in configuration space from the $m = 0$ packings [Fig. 1(b)]. In contrast, the packings that occur at large μ approach the $m = 0$ packings in configuration space. Thus, we find that the lengths of the $m = 1$ lines increase with μ. $m = 2$ [Fig. 1(c)] and higher-order saddle packings populate areas and higher-order volumes in configuration space.

To determine the probability $P_m(\mu)$ that a packing occurs with maximum friction coefficient μ and saddle index m, we assume that the partition function $Z_m(\mu)$ is proportional to the configuration space volume, which contains solutions to the force and torque balance equations on each particle with tangential and normal forces that satisfy the Coulomb criterion and $F_{ij}^n \geq 0$. We calculate probabilities

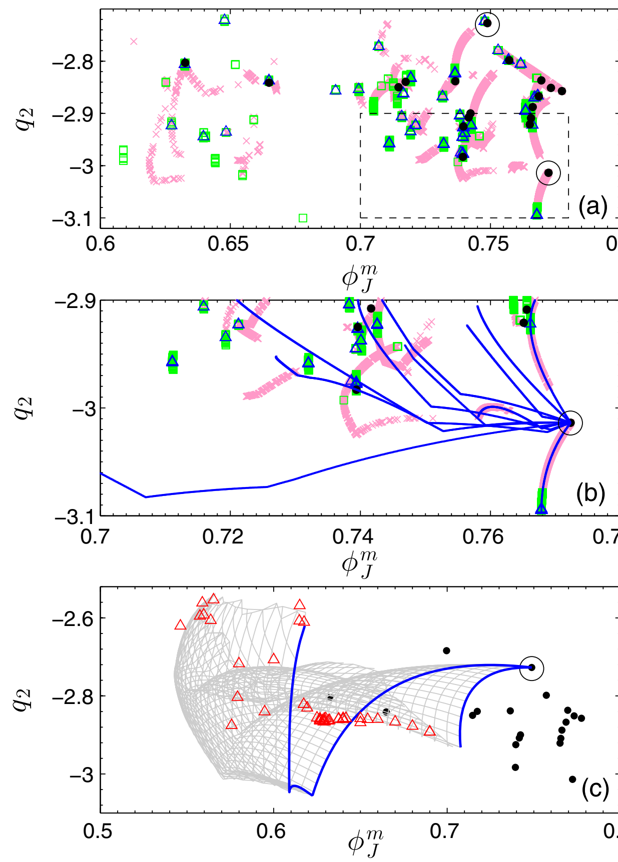

FIG. 1 (color online). (a) Second invariant q_2 of the distance matrix versus packing fraction at jamming onset ϕ_J^m for packings of bidisperse disks with $N = 6$ generated using the Cundall-Strack model for friction with $\mu = 0$ (filled circles), 0.002 (triangles), 0.02 (squares), and 0.2 (exes). Only packings with $m = 0$ and 1 are shown. (b) Close-up of boxed region in (a) with $m = 1$ packings (solid blue lines) generated using the spring network method that originate from the circled $m = 0$ packing. (c) $m = 2$ packings (gray mesh) that are generated from the two highlighted $m = 1$ families (solid blue lines) using the spring network method. $m = 2$ packings generated using the Cundall-Strack method that possess the same contact network as those from the spring network (gray mesh) are indicated by triangles. The $m = 1$ and 2 packings originate from the circled $m = 0$ packing.

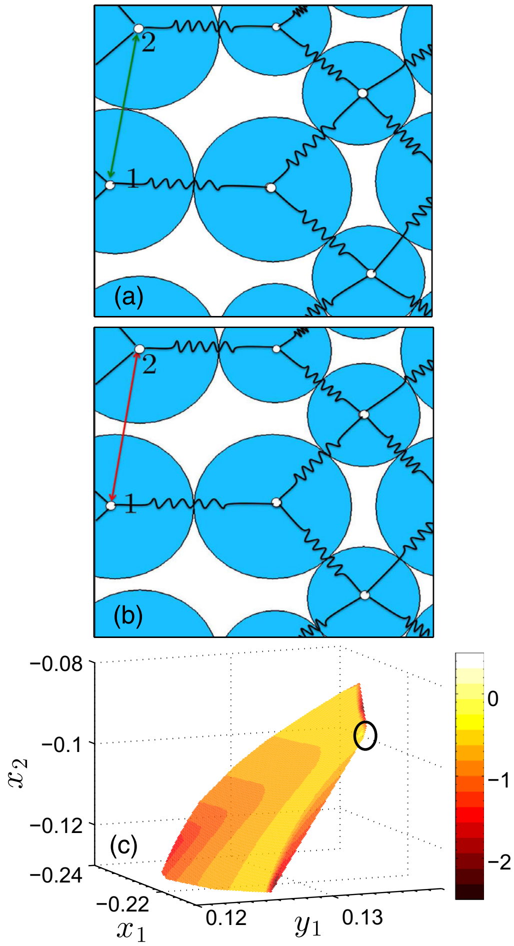

FIG. 2 (color online). (a) $m = 0$ packing of $N = 6$ bidisperse frictionless disks with $N_c = N_c^0 = 11$ contacts. To enumerate packings with $m = 1$, the contact between disks 1 and 2 is broken and constrained to have separation (b) $r_{12}/\sigma_{12} = \lambda > 1$, while the other ten contacts are maintained (visualized as springs) at $r_{ij} = \sigma_{ij}$. Our packing-generation process [6] is performed with these constraints to create an $m = 1$ packing at ϕ_J^1 with only ten contacts. This process is repeated as a function of λ and for the other ten contacting particle pairs. (c) Contour plot of the minimum friction coefficient $\mu_{\min}$ required to achieve force and torque balance for a branch of $m = 2$ packings in configuration space spanned by the central position of the spring (x_1, y_1) constraining the first broken contact and x component of the spring constraining the second broken contact x_2. The $m = 2$ branch of packings emanates from the circled $m = 0$ packing. The color scale for $\log \mu_{\min}$ increases from dark to light.

for packings to possess m missing contacts using the Gibbs assumption of equal probabilities.

In contrast, we have shown directly using MD simulations that the probability of finding a particular packing with $m = 0$ from random initial conditions violates the Gibbs equal-probability assumption [6]. The reason is that the volume of configuration space that determines the probability of a particular packing with $m = 0$ is the volume of the initial conditions that end up in that particular $m = 0$ packing (i.e., its basin of attraction [16]), not the volume in configuration space that the packing itself occupies. Packings with $m = 0$ are represented by points in configuration space with negligible volume.

It is the volume in configuration space of the saddle packings that determines the fraction of packings with a given m. (See the Supplemental Material [17].) In this case, the partition function

$$Z_m(\mu) \propto V_m(\mu)\delta^{2N-1-m}, \tag{1}$$

where $V_m(\mu)$ is the total volume in configuration space of all packings in mechanical equilibrium at μ with saddle index m. The length scale δ is the characteristic radius of the geometrical structure formed from the Minkowski sum of objects with dimensions $2N - 1 - m$ and m that surrounds each packing in configuration space and represents the uncertainty associated with finding the packings. We further assume that $V_m(\mu)$ can be described using a characteristic length scale $l(\mu)$, so that $V_m(\mu) \sim [l(\mu)]^m$. Thus, $Z_m(\mu)$ has dimensions of length raised to the $2N - 1$ power, which is the total dimension of configuration space. If we scale $Z_m(\mu)$ by the $m = 0$ value $Z_0(\mu)$, we obtain

$$\frac{Z_m(\mu)}{Z_0(\mu)} \propto \left(\frac{l(\mu)}{\delta}\right)^m. \tag{2}$$

Using this approach, we measure the volume of configuration space in units of the volume in configuration space of packings with $m = 0$. To directly measure $Z_m(\mu)/Z_0(\mu)$, we first employ the spring network method to generate a grid of points for each branch of saddle packings of order m. At each grid point characterized by $(x_1, y_1, \ldots, x_m, y_m)$, we determine the minimum friction coefficient $\mu_{\min}(x_1, y_1, \ldots, x_m, y_m)$ required to achieve mechanical equilibrium for that configuration, using Monte Carlo moves to search the null space of the force- and torque-balance matrix [20,21]. The allowed configuration volume is determined by integrating over the $\mu_{\min}$ contour [Fig. 2(c)], such that $\mu \le \mu_{\min}(x_1, y_1, \ldots, x_m, y_m)$ for a given mth order branch of saddle packings. The total allowed volume in configuration space for a given m and μ, $V_m(\mu)$, is obtained by summing the volumes over all mth order branches.

We show in Fig. 3 that $[V_m(\mu)]^{1/m}$ scales linearly with μ for $m = 1$ and 2. This scaling matches our intuition because the total volume of the force-torque null space is constrained by the Coulomb criterion for each contact (or dimension). As μ increases, the region of possible solutions increases linearly with μ in each dimension from zero at $\mu = 0$ to the total volume of the null space as $\mu \to \infty$. As $V_m(\mu)$ approaches the total volume of the null space, the scaling $V_m \sim \mu^m$ will break down since the total volume of the null space is finite [22]. However, this does not occur

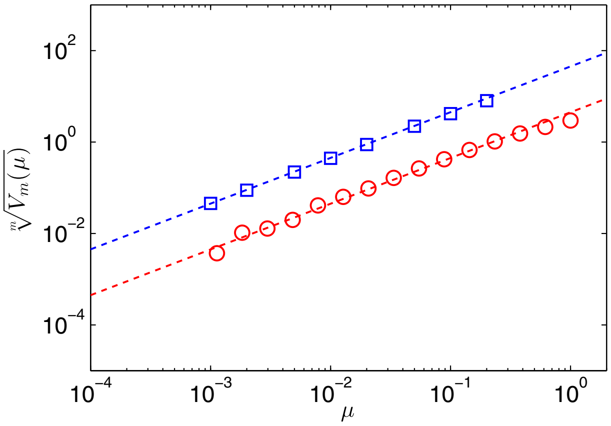

FIG. 3 (color online). mth root of the volume $V_m(\mu)$ in configuration space of the collection of mth order saddle packings ($m = 1$, squares; $m = 2$, circles) that are stabilized by a friction coefficient $\leq \mu$. The dashed lines have slope 1.

for the range of friction coefficients we considered ($\mu < 10$).

The normalized probability for an mth order saddle is

$$P_m(\mu) = \frac{Z_m(\mu)}{\sum_{m=0}^{m_{\max}} Z_m(\mu)} = \frac{A_m \mu^m}{\sum_{m=0}^{m_{\max}} A_m \mu^m} = \frac{a_m \mu^m}{1 + \sum_{m=1}^{m_{\max}} a_m \mu^m}, \tag{3}$$

where $a_m = A_m/A_0$ and the highest order saddle is $m_{\max} = (N-1)/2$ in 2D [23]. Assuming that the saddle packings at a given m occupy similar volumes in configuration space, a reasonable approximation for the coefficients is $A_m = c_m(N)N_s(N)N_b(N,m)$, where $N_s(N)$ is the number of $m=0$ packings for a given N and the normalized coefficients $a_m = c_m(N)N_b(N,m)$, where $N_b(N,m) = C_m^{N_c^0}$. We show in Fig. 4(a) that Eq. (3) with $c_m(N) = 1$ yields qualitatively correct results for the measured probabilities to obtain a given mth order packing from MD simulations of the Cundall-Strack model for $N = 30$ [Fig. 4(b)]. For example, $m = 0$ packings are most highly probable for small $\mu < 10^{-2}$, and the highest order saddles are most probable for $\mu > 1$. However, as shown in Fig. 4(b), we obtain a much better fit to the data from the Cundall-Strack model using

$$c_m(N) = \exp[-m(m - m_{\max})/m_{\max}], \tag{4}$$

which indicates an excess of mth order saddles for m near $m_{\max}/2$ that likely originates from rattler particles that exit or join the force-bearing network during compression. (See the Supplemental Material [17].)

We calculate the average contact number from $\langle z\rangle = 2(N_c^0 - \langle m\rangle)/N$. Our strategy is to use results for small systems (i.e., $N = 30$) to predict $P_m(\mu)$ and $\langle z\rangle$ versus μ for large N. We show in Fig. 4(c) that predictions from Eqs. (3) and (4) agree quantitatively with $\langle z(\mu)\rangle$ for $N = 64$ and 128 from the Cundall-Strack model. Thus, we have developed a method to calculate $\langle z(\mu)\rangle$ for large systems by enumerating frictional families in small systems.

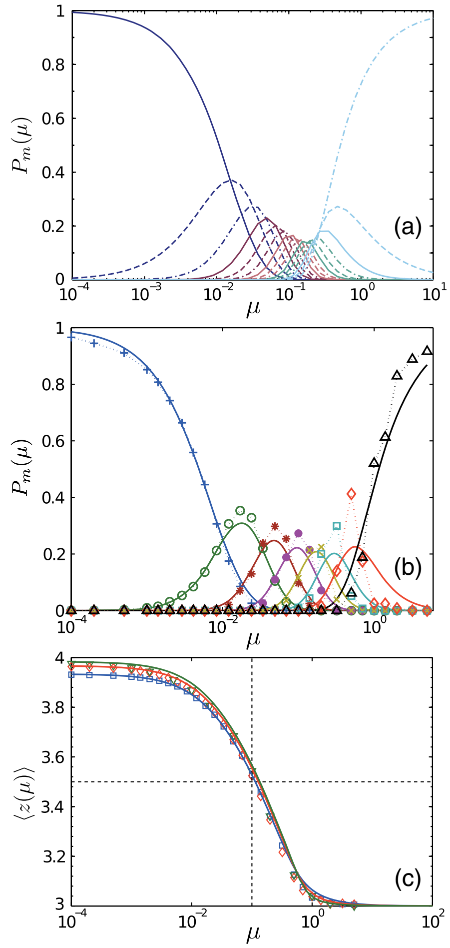

FIG. 4 (color online). (a) Probability $P_m(\mu)$ for a packing with $m = 0, 1, \ldots, 14$ (moving from left to right and dark to light) versus friction coefficient μ predicted by Eq. (3) with $c_m(N) = 1$ and $N = 30$. Each m has a different line type. (b) $P_m(\mu)$ for even m: $m = 0$ (pluses), 2 (open circles), 4 (asterisks), 6 (filled circles), 8 (exes), 10 (squares), 12 (diamonds), and 14 (triangles) from the Cundall-Strack model for $N = 30$ and fits to Eq. (3) (solids lines) with $c_m(N)$ from Eq. (4). The dotted lines are guides to the eye for the symbols. (c) $\langle z(\mu)\rangle$ for the Cundall-Strack model for $N = 30$ (squares), 64 (diamonds), and 128 (triangles) and fits to Eq. (3) (lines).

This work provides a framework for addressing several important open questions related to frictional packings. For example, why does the crossover from the low- to high-friction limits in the average contact number and packing fraction occur near $\mu \approx 10^{-2}$ for disks [10,11] compared to 10^{-1} for spheres [8,10] for fast compression algorithms. In addition, using the methods described above, we can determine how the crossover from low- to high-friction behavior depends on the compression rate and degree of thermalization in the packing-generation protocol. Such calculations are crucial for developing the ability to design granular assemblies with prescribed structural and mechanical properties.

We acknowledge support from NSF Grant No. CBET-0968013 (M. D. S.) and DTRA Grant No. 1-10-1-0021 (C. S. O. and S. P.). This work also benefited from the facilities and staff of the Yale University Faculty of Arts and Sciences High Performance Computing Center and NSF Grant No. CNS-0821132 that partially funded acquisition of the computational facilities.

[1] H. A. Makse, D. L. Johnson, and L. M. Schwartz, Phys. Rev. Lett. **84**, 4160 (2000).
[2] L. Vanel, D. Howell, D. Clark, R. P. Behringer, and E. Clément, Phys. Rev. E **60**, R5040 (1999).
[3] D. Fenistein, J. W. van de Meent, and M. van Hecke, Phys. Rev. Lett. **92**, 094301 (2004).
[4] N. Xu, C. S. O'Hern, and L. Kondic, Phys. Rev. E **72**, 041504 (2005).
[5] K. To, P.-Y. Lai, and H. K. Pak, Phys. Rev. Lett. **86**, 71 (2001).
[6] G.-J. Gao, J. Blawzdziewicz, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. E **80**, 061304 (2009).
[7] L. E. Silbert, D. Ertas, G. S. Grest, T. C. Halsey, and D. Levine, Phys. Rev. E **65**, 031304 (2002).
[8] P. Wang, C. Song, C. Briscoe, K. Wang, and H. A. Makse, Physica (Amsterdam) **389A**, 3972 (2010).
[9] C. Song, P. Wang, and H. A. Makse, Nature (London) **453**, 629 (2008).
[10] L. E. Silbert, Soft Matter **6**, 2918 (2010).
[11] S. Papanikolaou, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. Lett. **110**, 198002 (2013).
[12] E. Somfai, M. van Hecke, W. G. Ellenbroek, K. Shundyak, and W. van Saarloos, Phys. Rev. E **75**, 020301(R) (2007).
[13] T. Bertrand, C. F. Schreck, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. E **89**, 062203 (2014).
[14] S. Henkes, M. van Hecke, and W. van Saarloos, Europhys. Lett. **90**, 14003 (2010).
[15] P. A. Cundall and O. Strack, Geotechnique **29**, 47 (1979).
[16] S. S. Ashwin, J. Blawzdziewicz, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. E **85**, 061307 (2012).
[17] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.113.128302, which also includes Refs. [18] and [19], for (1) the difference between "basin volumes" and the volume of configuration space occupied by mth order saddle packings and (2) the effect of rattler particles on the power-series expansion of the partition function in terms of the static friction coefficient.
[18] S. S. Ashwin, J. Blawzdziewicz, C. S. O'Hern, and M. D. Shattuck, Phys. Rev. E **85**, 061307 (2012).
[19] G.-J. Gao, J. Blawzdziewicz, and C. S. O'Hern, Phys. Rev. E **74**, 061304 (2006).
[20] T. Unger, J. Kertész, and D. E. Wolf, Phys. Rev. Lett. **94**, 178001 (2005).
[21] M. R. Shaebani, T. Unger, and J. Kertész, Phys. Rev. E **79**, 052302 (2009).
[22] To fix the dependence of $V_m(\mu)$ on the friction coefficient at large μ, we can choose $V_m(\mu) \sim \mu/[\mu/\mu_{\max}(m) + 1]$.
[23] If N is even, $m_{\max}$ is rounded down to the nearest integer.