journal ref.: Tamás Unger, Dietrich E. Wolf, János Kertész;
Force indeterminacy in the jammed state of hard disks,
Phys. Rev. Letters, **94**, 178001 (2005)

Force indeterminacy in the jammed state of hard disks

Tamás Unger
Dept. of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary and Institute of Physics, University Duisburg-Essen, D-47048, Duisburg, Germany

János Kertész
Dept. of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary

Dietrich E. Wolf
Institute of Physics, University Duisburg-Essen, D-47048, Duisburg, Germany

Granular packings of hard discs are investigated by means of contact dynamics which is an appropriate technique to explore the allowed force-realizations in the space of contact forces. Configurations are generated for given values of the friction coefficient, and then an ensemble of equilibrium forces is found for fixed contacts. We study the force fluctuations within this ensemble. In the limit of zero friction the fluctuations vanish in accordance with the isostaticity of the packing. The magnitude of the fluctuations has a non-monotonous friction dependence. The increase for small friction can be attributed to the opening of the angle of the Coulomb cone, while the decrease as friction increases is due to the reduction of connectivity of the contact-network, leading to local, independent clusters of indeterminacy. We discuss the relevance of indeterminacy to packings of deformable particles and to the mechanical response properties.

Jamming [1] has been in the focus of recent studies because it occurs in a great variety of phenomena like structural and spin glasses, colloidal systems, vehicular traffic and granular media. The characterization of the jammed state is therefore crucial and can perhaps be best achieved in granular systems. Many intriguing properties of granular packings originate from the microscopic force transmission through a contact structure, where non-linearity and disorder are known to be crucial. It is an essential but not resolved question how the highly inhomogeneous force-network influences the macroscopic stress transmission in dense granular media.

Since the deformations of the grains are usually much smaller than their size, a very useful reference system for granular matter is that of rigid (undeformable) particles [1–4]. It is known that random packings of frictional rigid disks or spheres exhibit a *hyperstatic* structure [5–7]: the number of the linear equilibrium equations of the grains, which relate the unknown contact forces to the external load, is too small to determine the contact forces uniquely. Therefore many mechanically admissible force-networks are possible in the same packing geometry and for the same external load, which define an *ensemble* of force-configurations.

This ensemble recently has received much attention [6, 8–14] due to the idea that some macroscopic properties of jammed granular systems can be derived based on an ensemble average over the admissible force-states [8]. The determination of force distribution in [9] or Green function in [10] are based on this approach.

Another interesting aspect of the force-ensemble is related to the behavior of the system under external perturbations. Packing structures where contact forces are unique or strongly restricted appear to be fragile: slight change of the load can cause rearrangements of the particles [15, 16]. The question arises whether a packing that exhibits many possible realizations of equilibrium forces becomes more robust against perturbations.

The results of this Letter provide nontrivial information also for packings of deformable particles: The actual network of contact forces (which is uniquely determined by the elastic deformations) must be contained in the force-ensemble calculated for the same contact geometry assuming the particles (in their deformed shape) would be perfectly rigid. Moreover, for a finite system of sufficiently rigid particles the contact geometry can be arbitrarily close to the ideal one obtained for perfect rigidity. Which of the solutions in the force ensemble is realized, depends e.g. on the elasticity of the individual grains. Here we address the question, how strong the restrictions provided by the force ensemble are.

Again another but closely related issue is that of hard particle simulations, where the dynamics is seemingly ambiguous due to the indeterminacy of forces [13].

The above problems indicate the significance of the force-ensemble, however very little is known about its properties. In this Letter some characteristics of the ensemble are revealed, where emphasis is put on the influence of friction.

In the recent literature [9, 10] it was suggested that all elements in the ensemble of admissible force configurations are realized with equal probability. This microcanonical approach can be regarded as a restricted version [23] of the Edwards ensemble [1–3]. In the following we also address the validity of this assumption.

Let us consider n rigid, cohesionless disks. A configuration of the contact forces $\{\mathbf{F}_i\}$ (where i is the contact index) is called admissible or a solution if two conditions are fulfilled: the *equilibrium* and the *Coulomb* conditions. The first one requires force and torque balance at each

grain, while the Coulomb condition reads:

$$|(\mathbf{F}_i)_t| \leq \mu\,(\mathbf{F}_i)_n \tag{1}$$

for the normal and tangential force at each contact, where μ is the friction coefficient. For $\mu > 0$ no additional condition is needed to exclude tensile forces.

Next we show that the solutions form a convex set. The space of contact forces $\mathcal{F}$ is defined (for fixed contact network) as an $N_c \times d$ dimensional vector space, where each point represents a force-configuration $\{\mathbf{F}_i\}$. N_c is the number of contacts, and d the space dimension (i.e. each contact force component represents one degree of freedom). Let $\mathcal{S}$ be the *subset of admissible states* in $\mathcal{F}$ under some fixed external forces. For a regular packing of disks $\mathcal{S}$ is known to be a convex polyhedron [11] but it is easy to see that *convexity is satisfied in any case*: shape of the particles, disorder, dimensionality or friction do not matter. Convexity means that if $\{\mathbf{F}_i\}$ and $\{\mathbf{F}_i + \Delta\mathbf{F}_i\}$ are solutions then $\{\mathbf{F}_i + \lambda\Delta\mathbf{F}_i\}$ is a solution as well for $0 \leq \lambda \leq 1$. First, the equilibrium condition holds: Both given force-configurations provide equilibrium against the external load, thus their difference $\{\Delta\mathbf{F}_i\}$ corresponds to zero load and exerts no total force or torque on the particles. Therefore it can be scaled freely (unrestricted λ) and added to an admissible state, that does not violate the linear equilibrium equations. Second, the Coulomb condition is satisfied simply because for each contact i the d-dimensional Coulomb "cone" is a convex set and therefore must contain the component $\mathbf{F}_i + \lambda\Delta\mathbf{F}_i$, with $0 \leq \lambda \leq 1$.

The solution set $\mathcal{S}$ reflects basically the properties of the contact-network, therefore when studying $\mathcal{S}$ it is crucial what kind of packing structure is considered. In real processes which lead to jamming, the microscopic structure is not prescribed but develops spontaneously up to the point, where further rearrangements against outer driving forces are blocked. This *self-organized* texture is an important feature of granular materials [15] which is disregarded in models using, e.g., regular arrangements [11, 12]. Therefore the packings studied below were constructed with discrete element simulations where the particles obeying Newton's dynamics build up the contact-network in a compression process. In these jammed configurations we search for various solutions of the contact forces and study the influence of friction on the properties of $\mathcal{S}$.

A detailed description of our method of constructing the packings and exploring admissible force-configurations can be found in [6], here only a short review is given. With the help of the contact dynamics algorithm [17, 18] a 2D system of 200 rigid disks is compressed along the vertical axis between two horizontal plates. Horizontally periodic boundary conditions are applied, gravity is set to zero, disk radii are uniformly distributed between R and $2R$, the horizontal system width is $42R$. We wait till the packing jams (relaxes into equilibrium) under the constant force of compression. Then, to avoid the effect of the straight plates, only the middle part of the static configuration is considered for further investigation: this is a horizontal slice of height $28R$ throughout the whole width in the bulk away from the plates. We retain the contact forces at the top and bottom perimeter of the slice as fixed boundary forces, thus they provide the external load on the system. The plates and the disks outside the slice can be left away.

After that the exploration of the admissible force-solutions follows for this fixed arrangement of disks. We start with the force state that appeared at the jamming and perturb all contact forces randomly [24], which leads out of equilibrium and violates the Coulomb condition. This perturbed state serves as the input for the Gauss-Seidel-like iterative solver of the contact dynamics method. This iterative algorithm lets the forces relax into a consistent state, providing a (possibly) new solution [6, 18]. The perturbation and relaxation can be repeated many times always starting from the last solution (a kind of random walk in the force space); in that way it is possible to *sample points* from $\mathcal{S}$.

Based on this collection of force solutions we can assess the differences between admissible states and study the problem of force indeterminacy. The main feature of $\mathcal{S}$ that we found in these self-organized structures is that the admissible force-networks are rather similar: The pattern of strong force lines changes little from one realization to the other, showing that the contact-network *imposes strong restrictions* on the force-configuration.

For each contact force $\mathbf{F}_i$ its variance $(\delta F_i)^2$ is calculated over the measured realizations. The ratio

$$\eta = \langle \delta F \rangle / \langle |\mathbf{F}| \rangle \tag{2}$$

represents the ensemble fluctuation in $\mathcal{S}$, thus it can be regarded as a *measure of ambiguity of the forces.* $\langle\cdot\rangle$ means the average over all contacts. The *force ambiguity* η has to be distinguished from the *degree of indeterminacy* which refers to the dimension of the affine subspace of force configurations solving the equilibrium conditions (without the restrictions due to the Coulomb cones).

To investigate the effect of friction a *new* packing is constructed for each value of μ before sampling the solutions. The force ambiguity η is plotted in Fig. 1 (full circles). Values of η around 10^{-7} reflect the accuracy level of our calculation and the corresponding force-configurations can be regarded as identical with this tolerance. In the zero friction limit the force ambiguity disappears *confirming isostaticity* of frictionless packings [7, 19, 20]. For small μ the force ambiguity grows proportionally with friction, however for larger μ it decreases again. The largest ambiguity of the forces is found around $\mu \approx 0.1$. Despite the further opening of the Coulomb angle fluctuations are getting smaller, even fully determined states are found for strong friction.

The behavior of η results from *two competing effects*: first, increasing friction provides larger freedom locally for the tangential forces, second, it also stabilizes the system in a less dense state [21] causing lower connectivity of the contact-network (open circles in Fig. 1), which

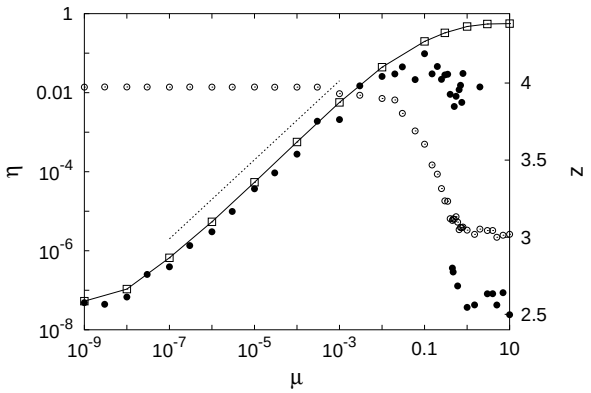

FIG. 1: Force ambiguity η (full circles) and average coordination number z (open circles) as functions of the friction coefficient μ. For comparison, squares connected by line show the η values for a configuration of disks that was constructed without friction.

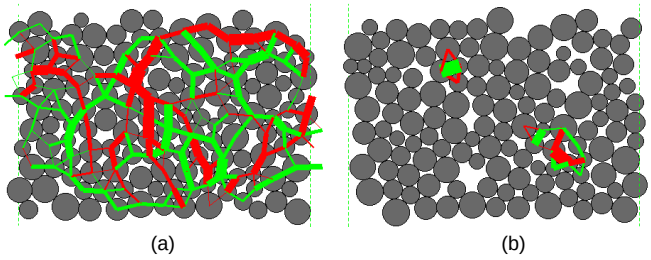

FIG. 2: (Color online) The difference between two admissible force-networks for (a) $\mu = 0.1$ (b) $\mu = 0.5$. Only normal force differences are indicated with different colors depending on their sign.

reduces force ambiguity. One can separate the two effects by fixing the configuration and letting the Coulomb angle alone influence η: We generated one packing without friction but switched on friction before sampling force-configurations. The results obtained this way (squares in Fig. 1) provide monotonously increasing fluctuations, as expected. Compared to the original data (full circles) deviations appear only on the right side of the figure, where the changes in the connectivity become important, while the behavior on the left side is governed by the first effect. For small μ the average coordination number of the configuration is essentially the same as in the frictionless case, where from isostaticity $N_c \approx 2n$ follows. This gives us the *degree of indeterminacy*: $2N_c - 3n \approx N_c/2$, since there are two unknown force components per contact and three equations per disk due to force and torque balance. Thus we conclude that for tiny friction there is a *small but high-dimensional* set of force-solutions in the $2N_c$ dimensional force-space, and its size goes to zero with vanishing friction. Similarly for spheres in three dimensions one obtains an N_c-dimensional solution set $\mathcal{S}$ within a $3N_c$-dimensional force space $\mathcal{F}$.

For large μ the dimension of $\mathcal{S}$ is strongly reduced due to the decreasing number of contacts. In our small system we found that $\dim(\mathcal{S})$ can reach even zero, allowing only one *single force-configuration*. This case corresponds to the marginal rigidity state found in experiments [22].

The regression of the degrees of freedom occurs in an interesting way: the *indeterminacy gets localized* in space into small subgraphs of the contact-network, which are surrounded by determined forces, i.e. a relatively large ambiguity is present but only in a small part of the system (Fig. 2.b). The pattern of the fluctuation-bearing contacts can be visualized by plotting the difference between any two admissible force-configurations. We found the same subgraphs as in Fig. 2.b also for other arrangements of boundary forces, showing that this indeterminacy-pattern is indeed a property of the packing texture. Each of the two subgraphs shown in Fig. 2.b is statically indeterminate, carries only one degree of freedom and cannot be reduced further because the deletion of one particle or one contact would cancel the internal indeterminacy. We call such subgraphs *elementary clusters*. They can be regarded as geometric units of indeterminacy.

If the connectivity is high the formation of elementary clusters is more probable, which suggest the following picture: For small friction many overlapping elementary clusters are formed so that two admissible solutions generically differ throughout the system (Fig. 2.a). As N_c is reduced the density of the elementary clusters ρ decreases and the indeterminacy gets localized into small separated domains. Around $\mu = 1$ the density ρ becomes so small that only a few elementary clusters are present due to the finite system size. This explains the strong scattering of the data for η in Fig. 1.

The spatial localization raises the question of a percolation transition. In case of small ρ the separated domains carry force-fluctuations *independently* of each other, therefore we think that η becomes a well defined intensive quantity for large systems. However if the indeterminacy percolates through the system the overlapping elementary clusters provide fluctuating boundary forces for each other, thus the indeterminacy of forces is enhanced with growing system size. Simulations up to 500 particles show this *size dependence*, but it is not clear what happens in the thermodynamic limit.

Finally we investigate the dynamically created force-configuration $\{\mathbf{F}_{i,0}\}$, which is determined by the construction history. Our findings indicate that this state is *more "central"* than typical points in the solution set: We generate 20 initial configurations with $\mu = 0.01$ and sample for each of them 100 points randomly in $\mathcal{S}$. Their (vectorial) average is regarded as the center of $\mathcal{S}$. Then we measure the Euclidean distances ℓ of the sampled points from the center. The histogram of the distances in units of their average $\bar{\ell}$ is shown in Fig. 3 together with the histogram of the distances ℓ_0 of the initial, dynamically generated 20 points from the centers of the corresponding sets $\mathcal{S}$. The two histograms clearly indicate that the initial points are closer to the center on aver-

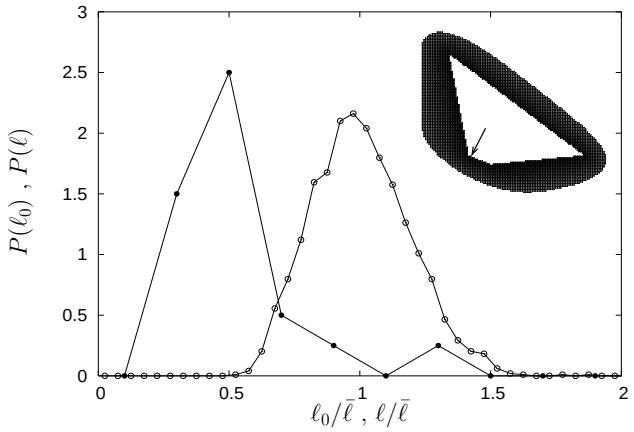

FIG. 3: Histograms of the distributions of normalized distances of dynamically generated (full circles) and randomly sampled (open circles) points in the sets $\mathcal{S}$ for $\mu = 0.01$. The inset shows a two dimensional cross section of a high dimensional solution set. The dynamically constructed force state is marked by the arrow. The white area belongs to $\mathcal{S}$, while outside $\mathcal{S}$ the gray scale indicates the violation of the Coulomb condition (darker means smaller violation).

age than the randomly sampled ones. Assuming that the distribution of the random sampling of $\mathcal{S}$ is close to a uniform one, we conclude that the force configurations of the dynamically generated jammed states are not uniformly distributed in the set $\mathcal{S}$.

That the original force configuration is "closer to the center" is not in contradiction to the fact that we always find it at the edge of two dimensional cross sections of the *high dimensional* solution set $\mathcal{S}$ (see inset of Fig. 3). We suggest the following physical picture: A contact with large mobilization of friction ($F_t/\mu F_n \approx 1$) is less stable against perturbations. Near the end of the relaxation process small collisions "shake" the already established contacts reducing the possibility that the contact remains on the verge of sliding. However, the system comes to rest finally by the marginal fulfillment of the Coulomb criterion at *some* contacts.

Our results show a significant difference between distributions of the solutions sampled by the random walks plus relaxation and of those relaxed physically. The uniformity of the (unbiased) random walk based sampling cannot be proved due to the high dimensionality of the problem, however, the distance distribution of the points should be rather robust just because of this high dimensionality. Therefore we consider the observed discrepancy though not as a proof but as a strong indication of the violation of the microcanonical assumption for the physically realized solutions.

It is expected that the ambiguity of forces for a given geometry has implications for the mechanical behavior. We regard the following preliminary result as an indication of such an effect. For a horizontal layer of hard disks settled under gravity we applied a point-force downwards on the free surface, just strong enough to cause local rearrangement. We measured the depth of the rearrangement zone and obtained non-monotonous dependence on μ: It is larger for small and large friction coefficients, and has a minimum at $\mu \approx 0.1$, right where η reaches its maximum.

This research was partially supported by DFG grant SFB 445, BMBF/OM grant HUN 02/011, OTKA T035028, and the Center for Applied Mathematics and Computational Physics of the BUTE.

[1] H. A. Makse, J. Brujic, and S. F. Edwards, in *The Physics of Granular Media* (Wiley-VCH, 2004), p. 45.

[2] S. F. Edwards and R. B. S. Oakeshott, Physica A **157**, 1080 (1989).

[3] A. Mehta and S. F. Edwards, Physica A **157**, 1091 (1989).

[4] F. Radjai, M. Jean, J. Moreau, and S. Roux, Phys. Rev. Lett. **77**, 274 (1996).

[5] L. E. Silbert, D. Ertas, G. S. Grest, T. C. Halsey, and D. Levine, Phys. Rev. E **65**, 031304 (2002).

[6] T. Unger and J. Kertész, Int. J. of Mod. Phys. B **17**, 5623 (2003).

[7] J. N. Roux, Phys. Rev. E **61**, 6802 (2000).

[8] J. P. Bouchaud, in *Slow Relaxations and Nonequilibrium Dynamics in Condensed Matter* (Springer, 2003), p. 131.

[9] J. H. Snoeijer, T. J. H. Vlugt, M. van Hecke, and W. van Saarloos, Phys. Rev. Lett. **92**, 054302 (2004).

[10] S. Ostojic and D. Panja (2004), cond-mat/0403321.

[11] T. Elperin and A. Vikhansky, Physica A **260**, 201 (1998).

[12] E. Clement, C. Eloy, J. Rajchenbach, and J. Duran, in *Stochastic Dynamics* (Springer, Berlin, 1998), p. 261.

[13] J. J. Moreau, in *Proc. of the 4th ECCOMAS* (University of Jyväskylä, Finland, 2004), CD.

[14] S. McNamara and H. Herrmann, Phys. Rev. E **70**, 061303 (2004).

[15] M. E. Cates, J. P. Wittmer, J. P. Bouchaud, and P. Claudin, Phys. Rev. Lett. **81**, 1841 (1998).

[16] G. Combe and J. N. Roux, Phys. Rev. Lett. **85**, 3628 (2000).

[17] M. Jean, Comput. Methods Appl. Mech. Engrg. **177**, 235 (1999).

[18] T. Unger and J. Kertész, in *Modeling of Complex Systems* (AIP, Melville, 2003), p. 116, cond-mat/0211696.

[19] C. F. Moukarzel, Phys. Rev. Lett. **81**, 1634 (1998).

[20] A. V. Tkachenko and T. A. Witten, Phys. Rev. E **60**, 687 (1999).

[21] D. Kadau, G. Bartels, L. Brendel, and D. E. Wolf, Phase Trans. **76**, 315 (2003), cond-mat/0206572.

[22] R. Blumenfeld, S. F. Edwards, and R. C. Ball (2001), cond-mat/0105348.

[23] In Edwards' thermodynamic theory the ensemble average is taken over force- and also over packing-configurations.

[24] We add random tangential and normal components to the contact forces, which are chosen uniformly from $[-\langle F_n\rangle, \langle F_n\rangle]$, where $\langle F_n\rangle$ is the average normal force in the system.