International Journal of Bifurcation and Chaos, Vol. 20, No. 3 (2010) 897–903

DOI: 10.1142/S0218127410026186

THIRD ORDER LOOPS OF CONTACTS IN A GRANULAR FORCE NETWORK

ROBERTO ARÉVALO, IKER ZURIGUEL,
SERGIO ARDANZA TREVIJANO and DIEGO MAZA
Departamento de Física y Matemática Aplicada,
Facultad de Ciencias, Universidad de Navarra,
E-31080 Pamplona, Spain

Received November 14, 2008; Revised January 26, 2009

The existence of small order loops of contacts is presented as an intrinsic characteristic of force granular networks. Based on molecular dynamics simulations, it is proposed that the presence of these small order loops — and in particular third order loops of contacts — is important to understand the transition from fluid-like to solid-like behavior of granular packings. In addition, we show a close relationship between the development of third order loops and the small forces of the granular packing in the sense that almost all third order loops allocate a force component smaller than the average.

Keywords: Third order loops; granular network.

1. Introduction

The process of jamming in disordered systems such as gels, glasses, foams, and granular assemblies has attracted the attention of many physicists in the last few years [Liu & Nagel, 2001]. The reason seems to be the apparently common behavior that all these systems present near the jamming threshold [Liu & Nagel, 2001]. Some authors [Cates *et al.*, 1998] have proposed that the origin of the jammed state is the spontaneous development of internal structures as a response to external loads. Hence, the response of any of the former systems will be elastic with respect to a compatible load whereas incompatible loads — when the compression axis is different — will cause plastic rearrangements. Understanding how this internal organization is a consequence of an externally applied stress has become one of the main goals for the physics of disordered media.

A remarkable property of static granular packings is their highly heterogeneous force distribution [Liu *et al.*, 1995; Mueth *et al.*, 1998] which can be observed in Fig. 1(a). Direct observation of stresses in granular packings is possible using photoelastic discs illuminated through crossed polarizers [Behringer *et al.*, 1999; Zuriguel *et al.*, 2007; Zuriguel & Mullin, 2008]. The images thus obtained show that stress propagates in the form of filamentary structures or "chains" that conform to the so-called "force network". Indeed, it is widely accepted that these filamentary force chains develop spontaneously at the onset of jamming of granular materials. The main actors behind this complex organization are particle–particle interactions. The probability distribution for the interparticle normal forces $P(F)$ in granular materials has proved to be, in most cases, an exponential tail for forces higher than the average [Mueth *et al.*, 1998]. Yet it has been found that a qualitative change in the $P(F)$ allows to distinguish between flowing and jammed systems [Corwin *et al.*, 2005]. Moreover, a recent thorough experiment showed that the tail of the distribution is qualitatively different if the jammed configuration is obtained by isotropically shearing

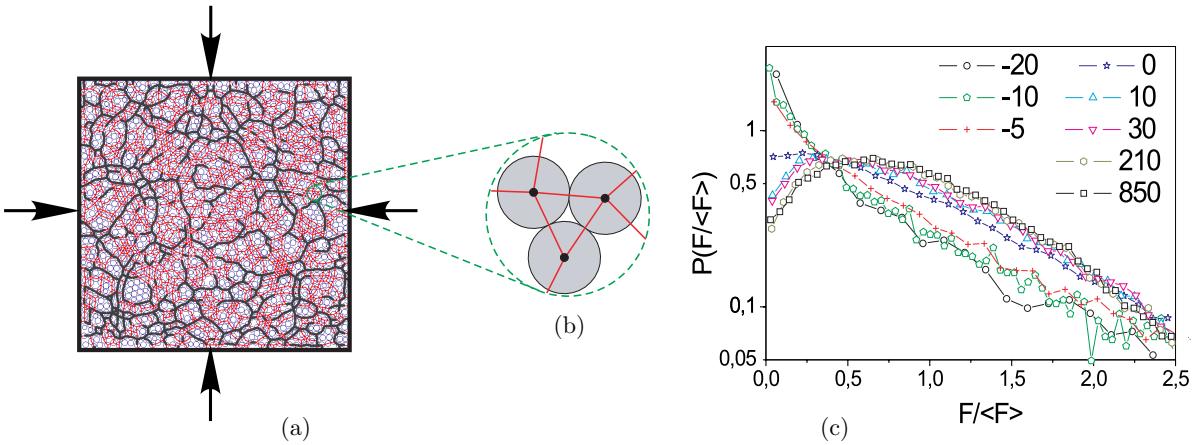


Fig. 1. (a) Schematic diagram of the numerical experiment. Discs are represented as circles and forces as red bonds. Superimposed gray bonds are the *edges* for the *graph* obtained for forces larger that the mean force. (b) Zoom of a third order loop inside the graph. (c) Normalized probability distribution function of the interparticle normal forces at the times (τ) shown in the legend.

or compressing the system [Majmudar & Behringer, 2005]. O'Hern *et al.* [2001] showed that the appearance of a well-defined maximum in the force distribution is also a distinctive signature of jamming in granular media. Other works show that $P(F)$ depends on the interparticle friction [Silbert *et al.*, 2002], and the hardness of the grains [Antony, 2002].

Alternatively to the shape of the $P(F)$, other parameters have been found to be related to the transition from fluid-like to solid-like behavior in granular media. Longhi *et al.* [2002] found a clear dynamical signature of jamming when granular media is flowing through an orifice. Specifically, they found that the distribution of time interval between collisions tends to a power law when the size of the orifice is reduced and the jammed state is attained. It is important to note that in this case, arrested states appear in the system as a sudden change in the dynamical state. Consequently, such transition is far from the "zero temperature" equilibrium states where many authors have developed a theoretical formalism to describe the jamming transition [O'Hern *et al.*, 2003]. Henkes and Chakraborty [2005], based on a mean-field approximation, proposed two order parameters that may characterize the transition from the jammed to the unjammed state: the average force per contact and the deviation of the average number of contacts from the isostatic value. This theory was in good agreement with the experimental results shown recently by Majmudar *et al.* [2007] who found a discontinuous increase in the mean contact number or coordination number Z at a critical volume fraction ϕ. This result is also in excellent accord with previous simulations [Silbert *et al.*, 2002; O'Hern *et al.*, 2002].

Despite these, and many other, important results, the mechanism by which a flowing media stops its dynamics and develops a collective arrested state is not yet well understood. The force distribution is intimately related with the topology, and the topology is related with the history of the grain assembly. The rigidity of a jammed state is undoubtedly determined by the existence of a *contact network* where loads, like information in a graph, propagates. Force and network interdependency has been studied by some authors under different assumptions [Jacobs & Thorpe, 1996; Mourkazel, 1998; Snoeijer *et al.*, 2004]. Recently an explanation for the origin of rigidity in a granular packing has been proposed by Rivier who represented a 3D granular packing as a graph with fixed length edges linking grains in contact and flexible hinges where the grains can rotate without sliding into each other [Rivier, 2006]. He found that the dynamical stability of granular materials was caused by the frustration arising from odd circuits or loops of contacts, whereas a material with only even circuits was not frustrated and constitutes a novel state of matter: a dry solid unable to resist shear.

In this work we explore the topological properties of the force network in the spirit proposed by Rivier [2007] and Ostojic *et al.* [2006]. Therefore, the contact topology is studied as a *graph* where particles are *nodes* and the interacting forces between them are *edges*. Under this scope we can asume that the force distribution inside the media is

defined by the history of the contact network. Thus, we study the development of small order loops of contacts near the onset of jamming. In particular, we focus on the study of the minimal loops of contacts i.e. third order loops where three particles contact each other and we show that most of the small forces of the network are allocated in these structures.

2. Numerical Method

We perform soft particle molecular dynamics simulations of the isotropic compression of a frictional granular sample consisting of 307 disks of radii R, and 1741 disks of radii $R_2 = (7/9)R$ in two dimensions with a linear interaction force. The values used for the parameters of the force model are: the frictional coefficient ($\mu = 0.5$), the elastic constant ($k_n = 10^5$), a dissipative coefficient $\gamma_n = 150$, and the corresponding ones for the tangential component ($k_s = \frac{2}{7}k_n$ and $\gamma_s = 300$) with an integration time step $\delta = 10^{-4}\tau$. The stiffness constants are measured in units of mg/R, the damping constants γ in $m\sqrt{g/R}$ and time in $\tau = \sqrt{R/g}$. Here, m and g stand, respectively, for the mass of the discs and the acceleration of gravity. The simulation protocol, which is explained in detail in [Arévalo *et al.*, 2006], has been shown to reproduce experimental results of the granular flow through an orifice [Mankoc *et al.*, 2007] and the arrangement of particles near a vertical wall in a semi-pile [Zuriguel *et al.*, 2008]. In this experiment, we consider only the horizontal case and therefore, there is no gravity acting on the system.

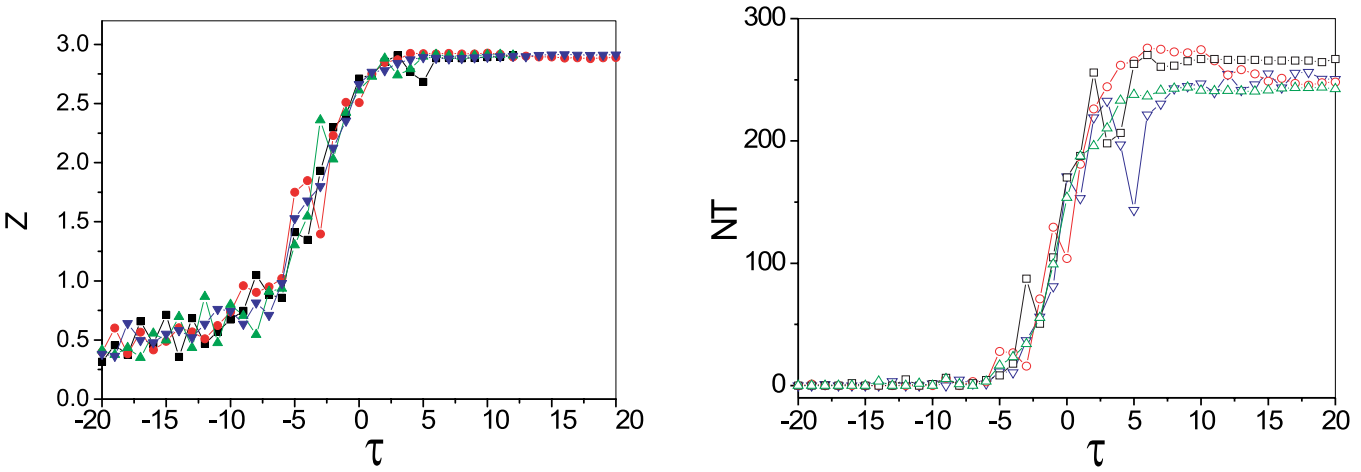
The simulation starts by setting the particles with random velocities and positions (drawn from a gaussian distribution) in a wide area. The test cell compresses the granular sample isotropically [Fig. 1(a)]. The compression is maintained by applying a force that increases constantly until a predefined value is attained. Alternatively other simulations have been carried out modifying some properties such as the system size, the sizes of the discs, the friction coefficient, the maximum compression and the geometry of the cell. Dependence of the results on these parameters was proven to be very small [Arévalo *et al.*, 2009]. We performed 20 simulations in order to average the results. In the following, triangular brackets $\langle \cdots \rangle$ are used to indicate mean values on each run and the averages obtained from the 20 simulations are indicated in bold type.

In order to achieve a better understanding of the origin of the jamming transition, the granular sample has been analyzed as a *force network graph* at each unit of time τ (10^4 simulation time steps). Graphs can also be built considering as edges only normal forces between grains that exceeds a threshold value f. Thus, grains are nodes only when they have, at least, a normal force above f. Hence, the network obtained for any force larger than zero is what we will call the *"contact network"*.

3. The Analysis of Third Order Loops

It is widely known that when a sample of grains is compressed there is a transition from fluid-like to solid-like behavior. In this paper, we check this transition analyzing the evolution of several variables as the simulation is carried out. Let us arbitrarily define $\tau = 0$ as the time where the kinetic energy falls below 0.1% of the total energy. We found that there is a discontinuity in the mean coordination number Z at $\tau = 0$ [Fig. 2(a)]. Other variables like the potential energy accumulated in the system or the number of contacts or edges also display a discontinuity at $\tau = 0$. In addition, the analysis of the $P(F/\langle F \rangle)$ for different τ reveals a qualitative change in the shape of the histogram before and after the jamming transition [Fig. 1(c)] in good agreement with [O'Hern *et al.*, 2001]. In the solid-like state ($\tau > 0$) a maximum of small forces appears in $P(F/\langle F \rangle)$ whereas in the fluid-like state ($\tau < 0$) the force distribution displays a monotonous decrease.

Let us now concentrate on the properties of the network before and after the transition from fluid-like to solid-like behavior. Among all the properties of the force and contact network that can be studied [Boccaletti *et al.*, 2006], we focus here on the number of small order loops of contacts, and more specifically in the simplest of these structures: the third order loops of contacts or triangles. A third order loop is defined as a three-step walk where the first and third nodes are the same [Fig. 1(b)]. Triangles are important because they are the minimal subgraph that satisfy the Laman rigidity theorem in 2D [Laman, 1970]. Accordingly, third order loops are the minimal odd circuits that provide rigidity to the developed "fragile" jammed state [Rivier, 2006]. The number of these loops is given by the clustering coefficient $C = \bar{C}_i$ times the number of nodes with $C_i = 2l_i/k_i(k_i - 1)$, where l_i is the number of

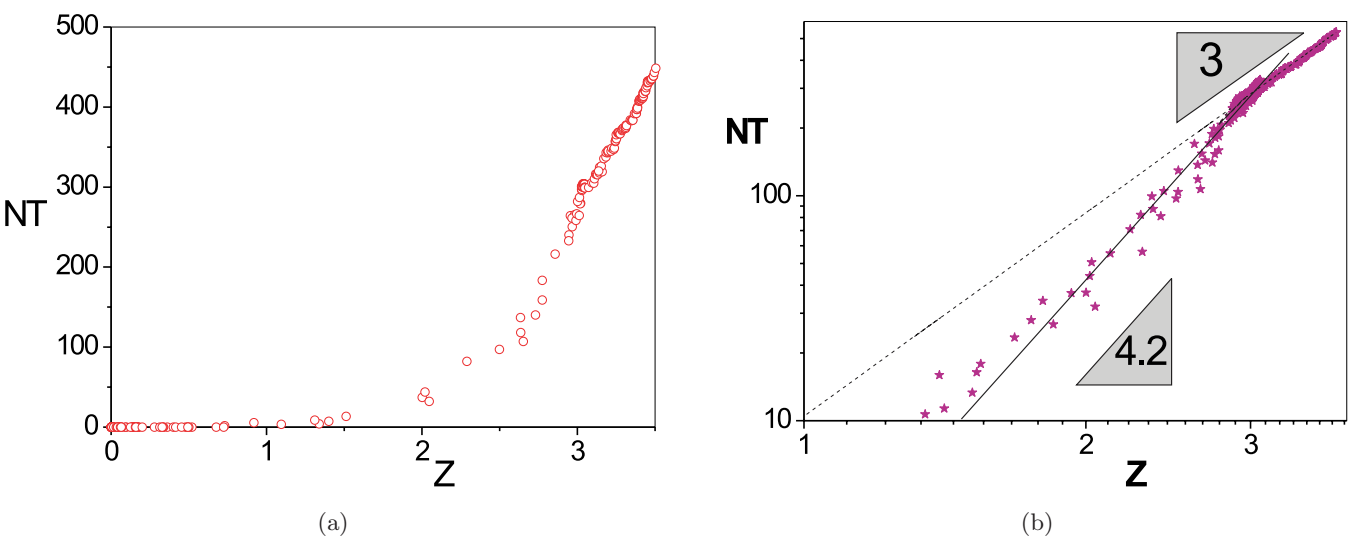


(a) (b)

Fig. 2. (a) Mean coordination number of the contact network versus time. Different symbols represent the data obtained for different runs. (b) The number of third order loops versus time.

edges between the neighbors of node i, and k_i is its number of neighbors [Costa *et al.*, 2007]. Another way to obtain the number of third order loops is by using the third moment of the adjacency matrix [Goh *et al.*, 2001].

The evolution of the number of triangles for different times is presented in Fig. 2(b). The first result that becomes evident is that the number of triangles suddenly grows at $\tau = 0$. Furthermore, the transition in the number of third order loops is more abrupt than the transition for the connectivity. This fact is displayed in Fig. 3(a), where the number of third order loops for a typical run is shown as a function of Z. Hence, it may be stated that the existence of third order loops is a property of rigid granular media since its number is almost zero when the granular media is deformable and takes a finite value when the media behaves like a solid. Third order loops are connected between them by higher order loops which eventually could suffer internal rearrangements if an annealing process would be applied. In any case, a further increase of the packing fraction will imply a larger number of three particles contacting each other and therefore, third order loops will be present in any jammed state developed by a disorder media.



(a) (b)

Fig. 3. (a) Number of third order loops versus the mean coordination number Z of the "contact network" for a single run. (b) Number of third order loops (**NT**) as a function of **Z**. The crossover between $\mathbf{NT} \propto \mathbf{Z}^3$ and $\mathbf{NT} \propto \mathbf{Z}^{4.2}$ allows us to calculate with good accuracy the critical value of the coordination number Z_c.

An interesting question that may arise when the results of Fig. 3(a) are considered is the interdependence between the number of third order loops NT and the number of contacts which define the average coordination number of the network (Z). Indeed, it seems reasonable to speculate about the possibility that the increase in the number of third order loops is just a consequence of the increase of Z. In the following, we answer this question by introducing a probabilistic approach.

Consider the final graph as an empty network, the dependency of the number of triangles as a function of the number of edges can be calculated. Given a polygonal configuration with E edges and V vertices (or nodes), as for instance, a triangular lattice with finite boundary, we can calculate the probability of obtaining k triangles when selecting randomly "e" edges and therefore, the expected number of triangles obtained.

Defining a triplet as any subset of three edges of the network, there are $N_{\text{trip}} = \binom{E}{3}$ possible triplets in the network. The probability that a triplet corresponds to a triangle of our network is $p = (NT_{\max}/\binom{E}{3})$, where $NT_{\max}$ is the total number of triangles present in the graph. On the other hand, selecting e edges is equivalent to selecting $n = \binom{e}{3}$ triplets. Then $m = NT_{\max}$ is exactly the number of triplets that form triangles. Hence, the random variable $XT =$ *number of triangles obtained after selecting* n *edges*, follows a hypergeometric distribution $P(XT = k) = f(k, N_{\text{trip}}, m, n)$:

$$f(k, N_{\text{trip}}, m, n) = \frac{\binom{m}{n}\binom{N_{\text{trip}} - m}{n - k}}{\binom{N_{\text{trip}}}{n}},$$

$$\max(0, n + m - N_{\text{trip}}) \leq k \leq \min(m, n) \qquad (1)$$

The expectation is given as $E(XT) = n(m/N_{\text{trip}})$ which in our original formulation in term of vertices and edges is

$$E(XT) = \binom{e}{3}\frac{NT_{\max}}{\binom{E}{3}} = NT_{\max}\frac{e(e-1)(e-2)}{E(E-1)(E-2)}$$

Provided that Z is a linear function of e ($Z = 2e/V$) we expect NT to grow with the coordination number as $NT \propto Z^3$ when the graph is randomly filled. This dependence of NT on Z is clearly observed in the numerical experiments for the values of Z corresponding to $\tau > 0$ [Fig. 3(b)] and has also been reported in tilted two-dimensional granular packings [Smart & Ottino, 2008]. However, before this period, the growth rate of **NT** is clearly larger than $\mathbf{Z}^3$ and a well-defined crossover can be identified. Note that in this case we refer to averaged values. As can be observed in Fig. 3(a), each particular run displays some dispersion in the values of NT before jamming which may depend on the initial conditions. On the contrary, all the simulations describe exactly the same dependence for $\tau > 0$ with no evidence of such dispersion. The result shown in Fig. 3(b) indicates that above the transition from fluid-like to solid-like behavior the new contacts in the network form third order loops as in a random graph and then $\mathbf{NT} \propto \mathbf{Z}^3$. On the contrary, before the transition, there is a growth in the number of triangles sharper than the expected $\mathbf{NT} \propto \mathbf{Z}^3$.

The crossover between both relationships of **NT** with **Z** allows us to estimate with good accuracy the critical coordination number Z_c at which the jamming transition takes place. This is indeed one of the most difficult tasks when proving the critical behavior of such a transition. From the results of Fig. 3(b) we obtain that $Z_c = 3.04 \pm 0.1$ for this particular configuration.

Once the number of third order loops has been shown to display a characteristic behavior in the transition to a rigid state, let us analyze its relationship with the force distribution on the network. In Fig. 4, **NT** is displayed for the final jammed state as a function of $f/\langle F\rangle$: the force threshold above which forces are considered to build the network (f) normalized by the mean force ($\langle F\rangle$). It is evident that when f is increased, the dilute graph contains a

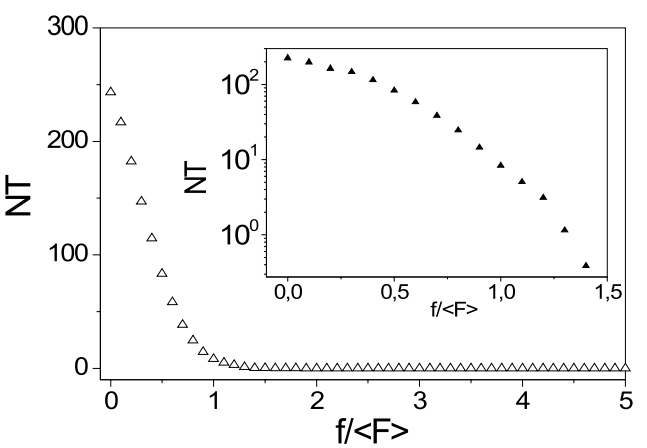


Fig. 4. Number of third order loops (**NT**) in the force network of a jammed state ($\tau = 850$) for different force thresholds ($f/\langle F\rangle$). Inset: a semilogarithmic plot of the same results.

significantly lower number of third order loops. In fact, **NT** shows a clear cut off as a function of f (see inset of Fig. 4). It is also remarkable that for a force threshold equal to the average, the dilute network contains less than 5% of the third order loops in the contact network. Consequently it can be stated that 95% of the triangles include, at least, a force smaller than the average. We speculate that this result is closely related to the idea introduced by Radjai *et al.* [1996] about the presence of two force subnetworks: a "load-bearing" percolating network carrying a force larger than the average, and a "dissipative" network carrying a force smaller than the average. Hence, the load-bearing network would be a subgraph with no small order loops whereas the "dissipative" network could be a subgraph formed basically by small order loops [Arévalo *et al.*, 2009].

In order to test the assumption that third order loops carry small forces of the network, we introduce P_T, the probability to find a force of magnitude $F/\langle F\rangle$ in a third order loop of contacts. The values of these probabilities for different τ are displayed in Fig. 5. Certainly for $\tau < 0$, P_T is near zero for all $F/\langle F\rangle$ as there are no third order loops in the contact network. Nevertheless, after the jamming transition P_T is a monotonic decreasing function of F. Indeed P_T reaches values larger than 0.6 when $F/\langle F\rangle$ tends to zero. This value is considerably higher than 0.269 which is the probability that an edge of the contact network belongs to a third order loop of contacts and hence, the expected value for P_T if the forces were randomly distributed within the final graph. Thus, a conclusion can be drawn in the sense that third order loops, which are intrinsically rigid, are able to catch the small forces of the network. Accordingly, the presence of third order loops in the network should have a strong influence in the shape of the probability distribution for the interparticle normal forces $P(F)$. This idea is in good agreement with the fact that before jamming — when there are no third order loops in the graph — $P(F)$ decreases monotonically, whereas after the jamming transition — when there are third order loops of contacts in the network — the probability function displays a peak and different laws are necessary to fit the profile.

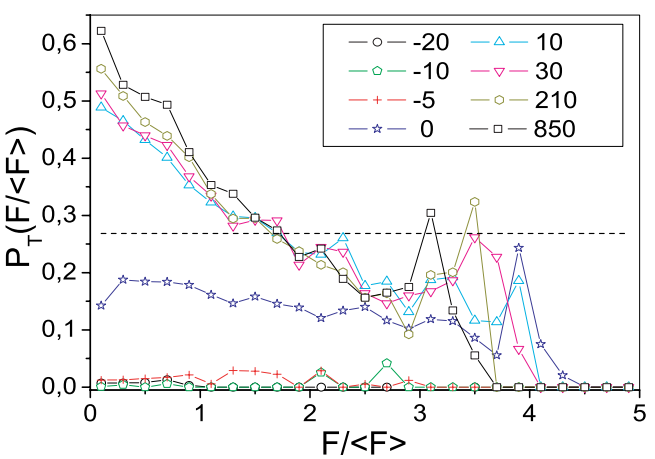


Fig. 5. Probability that a force ($F/\langle F\rangle$) falls into a third order loop of contacts. Different symbols correspond to the probability for the force networks at different times (see legend). The dashed line represents the probability that an edge belongs to a third order loop of contacts in the final jammed state (0.269).

4. Conclusions

In this work we show that the development of small order loops in the contact network is a key ingredient in the jammed state of granular materials. Additionally, we have found a clear relationship between the triangular arrangements of particles and the small forces in the network. Such observation has an important practical consequence: experimental methods need to determine univocally the topology of the small forces between particles in order to understand completely the jamming transition. A careful experimental evaluation of the interdependence between topology and small forces could give an explanation of the rigidity developed by a jammed ensemble. The role that parameters like friction or hardness of the grains have in the development of third order loops and their relative magnitude with respect to other small order loops is still unresolved. Preliminary results show similar global behavior with higher number of third order loops in the jammed state when these parameters are reduced.

Acknowledgments

This work was supported by project FIS2005-03881 (MEC, Spain) and PIUNA (University of Navarra). R. Arévalo thanks Asociación de Amigos de la Universidad de Navarra for a Scholarship. The authors are grateful to A. Garcimartín for helpful discussions concerning this work.

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