Complex force network in marginally and deeply jammed solids*

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This paper studies the force network properties of marginally and deeply jammed packings of frictionless soft particles from the perspective of complex network theory. We generate zero-temperature granular packings at different pressures by minimizing the inter-particle potential energy. The force networks are constructed as nodes representing particles and links representing normal forces between the particles. Deeply jammed solids show remarkably different behavior from marginally jammed solids in their degree distribution, strength distribution, degree correlation, and clustering coefficient. Bimodal and multi-modal distributions emerge when the system enters the deep jamming region. The results also show that small and large particles can show different correlation behavior in this simple system.

Keywords: jamming, complex networks, amorphous solids

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1. Introduction

Granular materials are intriguing because they exhibit many interesting phenomena such as force chains,[1] surface waves,[2] segregation,[3–6] granular clock,[7–10] granular packing,[11,12] and granular flow.[13–16] Granular materials, colloids, foams, and emulsions undergo a "jamming" transition from liquid to amorphous solid so that the constitutive particles cannot move freely.[17–19] At zero temperature and zero applied stress, the jamming transition occurs at a critical volume fraction ϕ_c (labelled as point "J").[20,21] When the volume fraction ϕ is near ϕ_c, many of the material properties are known to scale with a power-law dependence on $(\phi - \phi_c)$.[22–25] This is classified as a "marginally jammed state". However, when the volume fraction increases away from point J to a crossover volume fraction ϕ_d, the system enters a "deeply jammed state".[26] The scalings and density of states are all different from those in marginally jammed solids. The pair distribution function $g(r)$ also shows fundamental changes.

Figure 1 shows typical packs of a marginally jammed system and a deeply jammed system. One can see that there is a fundamental topological difference in their contact configuration. An extraordinary difference is: in the marginally jammed system the particles are in contact with their spatially nearest neighbors, while in the deeply jammed system the particles are in contact with their spatially nearest and next nearest neighbors. Although some structural characteristics of these two states can be detected with $g(r)$, it is valuable to investigate the topological property differences from the perspective of complex networks. Since the discovery of small-world and scale-free properties,[27,28] the complex network theory has made great progress.[29,30] The literature is replete with statements about contact networks and force chains[1] but the structural properties of a jammed system was investigated mainly by the pair distribution function $g(r)$. Recently, some efforts have been made to consider granular assemblies as complex networks.[31–35] The force network of a jamming system can be viewed as a special kind of complex spatial network. The models of spatial networks can be classified into five classes:[30] (i) geometric networks (including Apollonian networks[36]), that is, a set of vertices located in the space with edges constructed according to some geometric conditions; (ii) spatial Erdös–Rënyi random graphs: connecting nodes with some probability; (iii) spatial small-world networks: spatial variants of the Watts–Strogatz small-world network model;[28] (iv) spatial scale-free networks: spatial extensions of the Barabasi–Albert scale-free network model;[27] (v) optimal spatial networks: planed networks with a minimized "cost" function.

In this paper, we report our findings on the force network properties of marginally and deeply jammed solids from the perspective of complex networks. The force network can be seen as a model of optimal spatial network, since the granular packing is generated by minimizing the potential among the particles. A network possessing a power-law degree distribution is notable because there exists a small portion of nodes with a very high degree. In a granular system, it is unlikely that the degree distribution of the force network will be scale-free unless the particle size and shape distributions are widely ranged.[36] We show that there are fundamental differences between a marginally jammed solid and a deeply jammed solid. The degree distribution, strength distribution, degree correlation, and cluster coefficients are very different in the two solids.

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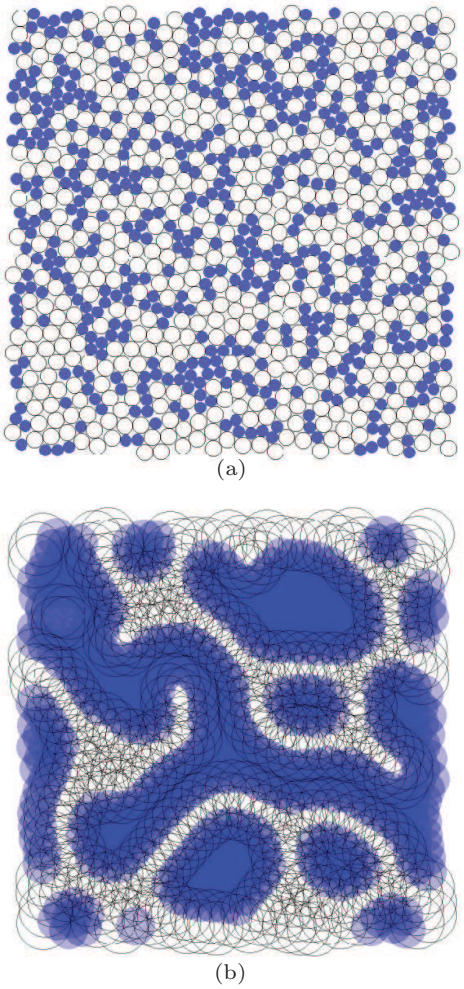


Fig. 1. (color online) Typical two-dimensional (2D) Hertzian packings of a marginally jammed state (a), $P = 0.001$ and a deeply jammed state (b), $P = 10.0$. Blue solid disks are small particles with diameter σ and black hollow ones are big particles with diameter 1.4σ.

2. Numerical method

We perform 2D and three-dimensional (3D) molecular dynamic simulations of soft disks/spheres packings. Although numerical simulations on 2D and 3D packings are done, this paper mainly contains 2D results. The system consists of a 1:1 binary mixture of $N = 1000$ frictionless disks/spheres interacting via springlike repulsive potential:[37]

$$V(r_{ij}) = \frac{\varepsilon}{\alpha}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^{\alpha}, \qquad (1)$$

when the center distance of particles i and j, r_{ij} is less than the sum of their radii, $\sigma_{ij} = (\sigma_i + \sigma_j)/2$, and 0 otherwise. It means that the interactions are finite in range, that is, particles do not interact unless they overlap. Potentials of this form were motivated by granular materials where particles have a well-defined diameter and do not interact except for a strong repulsive force. The diameter ratio of the two species is 1 : 1.4 to avoid crystallization.[21,22] The exponent $\alpha = 2.0$ is for repulsive harmonic springs, $\alpha = 2.5$ is for repulsive Hertzian interactions that are softer than harmonic springs. In our simulation, both Hertzian (HZ) and harmonic (SP) interactions are considered. We set the small particle diameter σ, particle mass m, and ε to be one. Thus the time is in the units of $\sqrt{m\sigma^2/\varepsilon}$.

The simulation starts with randomly placing the particles in a box or cube with random initial velocities, so that the initial system corresponds to an infinitely high temperature state. The initial volume fraction is set to be close to that at the desired pressure. Periodic boundary conditions are applied in all directions. Then the system is quenched to the local minimum of inter-particle potential energy by applying the $L-BFGS$ energy minimization method.[38] If the pressure of the output jammed state is higher (lower) than the desired value, the volume fraction is decreased (increased) by a small amount $\delta\phi$. The $L-BFGS$ method is applied again. This process of expanding/shrinking with a $L-BFGS$ energy minimization is applied successively until a jammed packing at the desired pressure P is obtained. At each pressure, we generate 50 distinct jammed configurations and take averages over their contact force networks. The pressure of the systems studied ranges from $P = 10^{-5}$ to $P = 10.0$. At $P \approx 0.2$ and $\phi_d \approx 1.68$ (2D), the system enters a deep jamming region.

3. Numerical results

We first define our granular force network, i.e., a set of nodes connected by links. Here every node corresponds to a particle and each link connects the pair of particles in contact. The normal forces between the particles are stored as the weight of the link. The tangential forces between the contacting particles are not considered.

3.1. Degree distribution

In a network or graph, degree (K) is the number of links connecting to the node, the same as the coordination number. The degree distribution is the distribution function of contact number per particle in the system.

Figure 2 shows the degree distributions. In a marginally jammed system, the distribution has only one peak, while it becomes bimodal for a deeply jammed system. In the marginally jammed region, the peak is found at $K = 4$ or $K = 5$ and most particles have $3 \sim 7$ contacts. There are a small portion of particles with $K = 0$ (rattlers). Note that our simulation excludes the configurations with any particle's degree lying between 1 and 2 because these particles are not stable. When the system enters a deep jamming region, the rattlers disappear. Then the degree distribution becomes bimodal and the gap between the two peaks grows with pressure. At $P \approx 5.0$, the curve becomes two separated peaks. Similar behavior is exhibited with the harmonic system. Because the Hertzian contact is softer, one can see that the range and peak positions of degree distribution are higher in comparison with the Hertzian system for the same pressure.

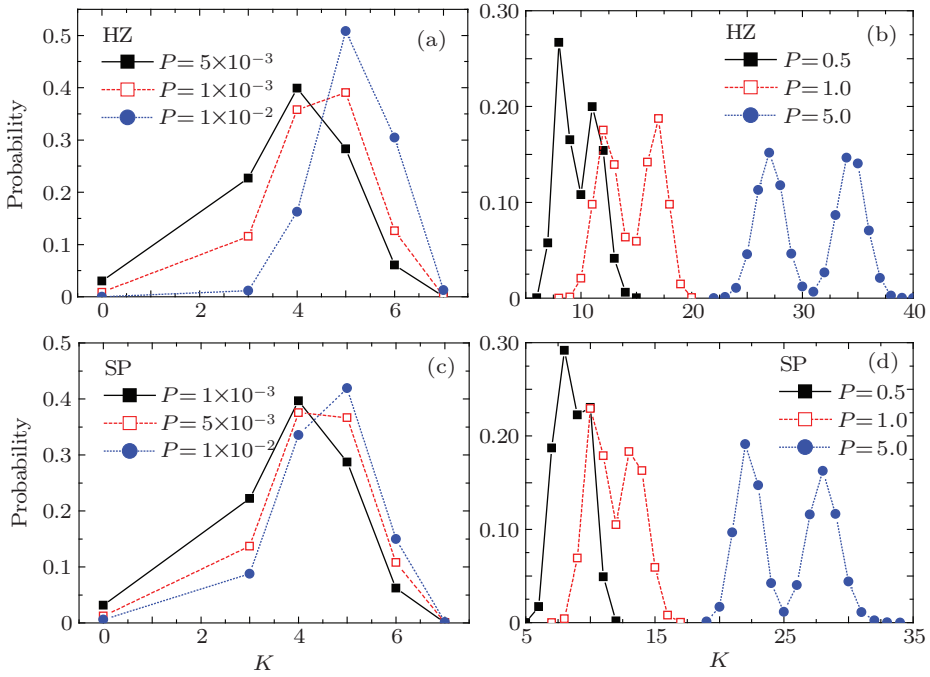


Fig. 2. (color online) Degree distribution for typical Hertzian (HZ) and harmonic (SP) systems. Panels (a) and (c): marginally jammed systems; (b) and (d) deeply jammed systems.

The emergence of a bimodal degree distribution is due to the bi-disperse nature of the system. The first peak is for the small particles, and the second is for the big particles. We checked this by examining the degree distribution of big and small particles separately. As show in Fig. 3(a) and 3(b), in both marginally and deeply jammed systems, the big particle has more contacts with others, while the small particle has less. But the average degrees of small and big particles are very close in a marginally jammed system, while they take quite different values in a deeply jammed system, as shown in Figs. 3(c) and 3(d). Therefore, the system's overall degree distribution becomes bimodal in a deeply jammed system. We have also studied a poly-disperse system where the particle diameter distributes uniformly from σ to 1.4σ. The degree distribution keeps unimodal for both marginally and deeply jammed systems.

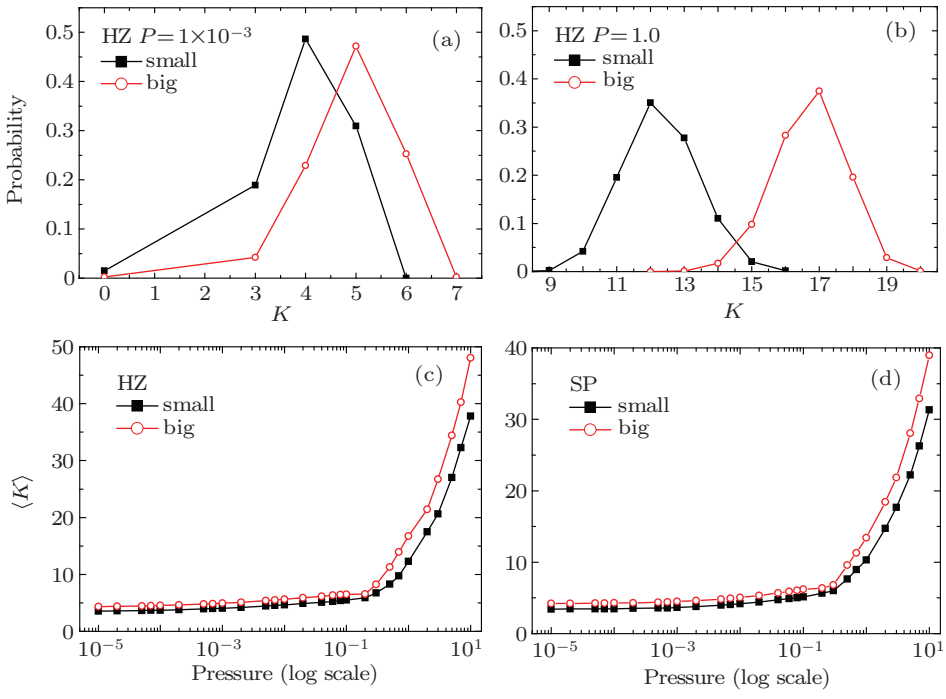


Fig. 3. (color online) Typical degree distributions of small and big particles in a marginally jammed system (a) and a deeply jammed system (b). Average degree of big and small particles for the Hertzian system (c), and for the harmonic system (d).

3.2. Strength distribution

Then we consider the node's strength. In the network language, node strength is defined as the sum weight of links connecting to the node. Here the weight represents the normal force between the particles. Thus the node strength can be used to evaluate the burden of particles.

Figure 4 shows the strength distribution of typical jamming systems. It roughly follows a Poisson distribution for the marginally jammed system. With the increase of pressure, the peak also changes to a higher strength. For the deeply jammed system, the strength becomes bimodal and then multi-modal. For harmonic systems, similar behavior is found, but it needs higher pressure to become multi-modal because the harmonic contact is harder.

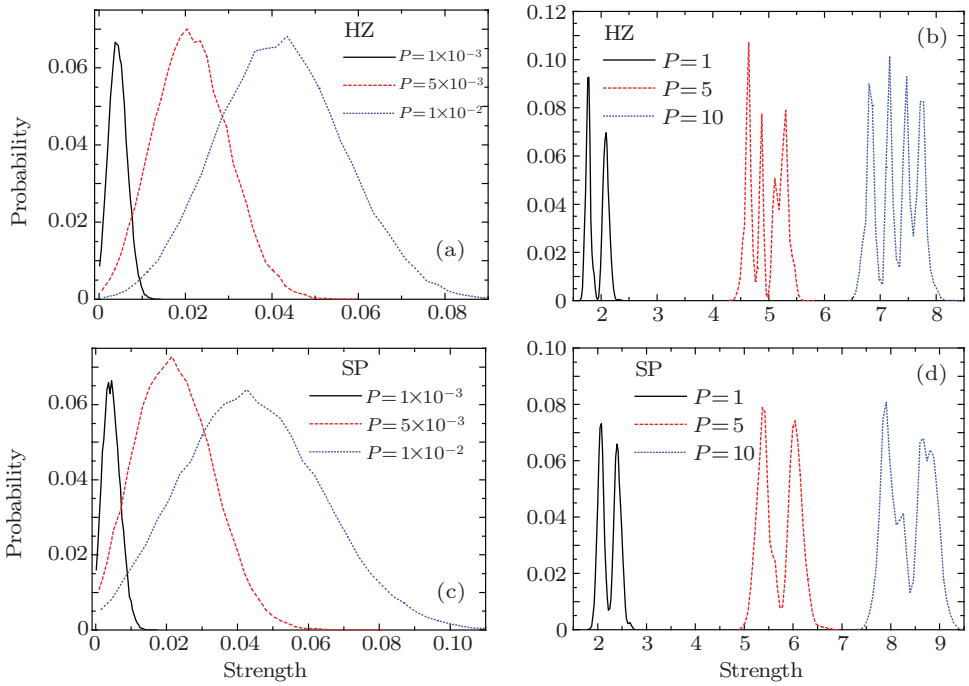


Fig. 4. (color online) Node strength distribution for typical Hertzian (HZ) and harmonic (SP) systems. (a) and (b) Marginally jammed systems and (c) and (d) deeply jammed systems.

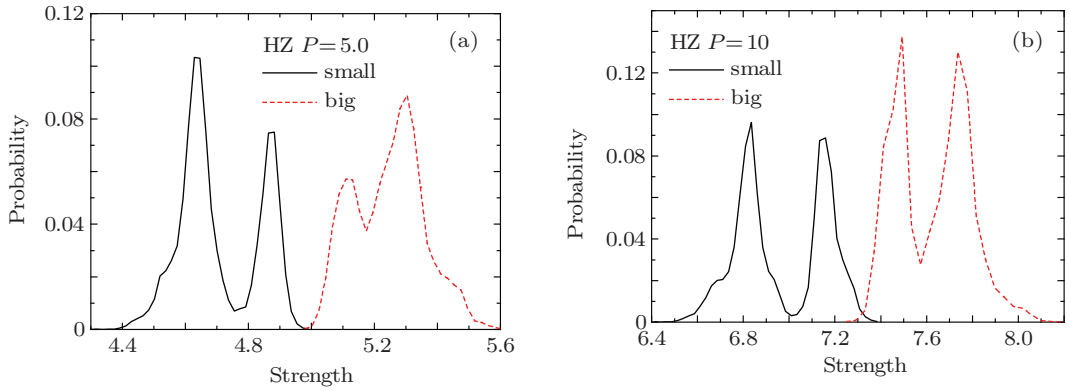


Fig. 5. (color online) Separated strength distribution for small and big particles in two typical deep jamming Hertzian (HZ) systems.

Similarly, the reason for bimodal strength distribution is due to the bidispersed nature of the system. To understand the multi-modal behavior, we separately examine the strength distribution for big and small particles. As shown in Fig. 5, the strength distribution becomes bimodal for both small and big particles with the increase of pressure. Since the strength distributions have peaks at different positions, the combination of small and big particles results in the multi-modal feature of the whole system.

3.3. Degree correlation

Now we consider the correlation behavior of the nodes in the system. Many real networks are correlated in the probability that a node of degree K is connected to another node of degree, say K', depending on K. The degree correlation can be evaluated by using the nearest neighbors' average degree

of node i as

$$K_{nn,i} = \frac{1}{K_i} \sum_{j \in N_i} K_j, \tag{2}$$

where the sum runs on the first neighbors of i. One can calculate the dependence of K_{nn} on node degree K, denoted as $K_{nn}(K)$. Correlated networks are classified as assortative if $K_{nn}(K)$ is an increasing function, whereas they are disassortative when $K_{nn}(K)$ is a decreasing function. In assortative networks the nodes tend to connect to the connectivity peers, while in disassortative networks low degree nodes are more likely connected with high degree ones.

Figure 6 shows $K_{nn}(K)$ for typical jamming systems. One can see that the system is disassortative in the marginally jammed region (Figs. 6(a) and (c)), while it becomes assortative for small particles and disassortative for big particles in the deeply jammed region (Figs. 6(b) and 6(d)). One can see that K_{nn} is an increasing function with the small particles ($22 \leq K \leq 30$ in Fig. 6(b)), while it is roughly a decreasing function with the big particles ($31 \leq K \leq 40$ in Fig. 6(b)). As far as we know, this is the first occasion to report on the nodes showing different correlation behavior in the same system.

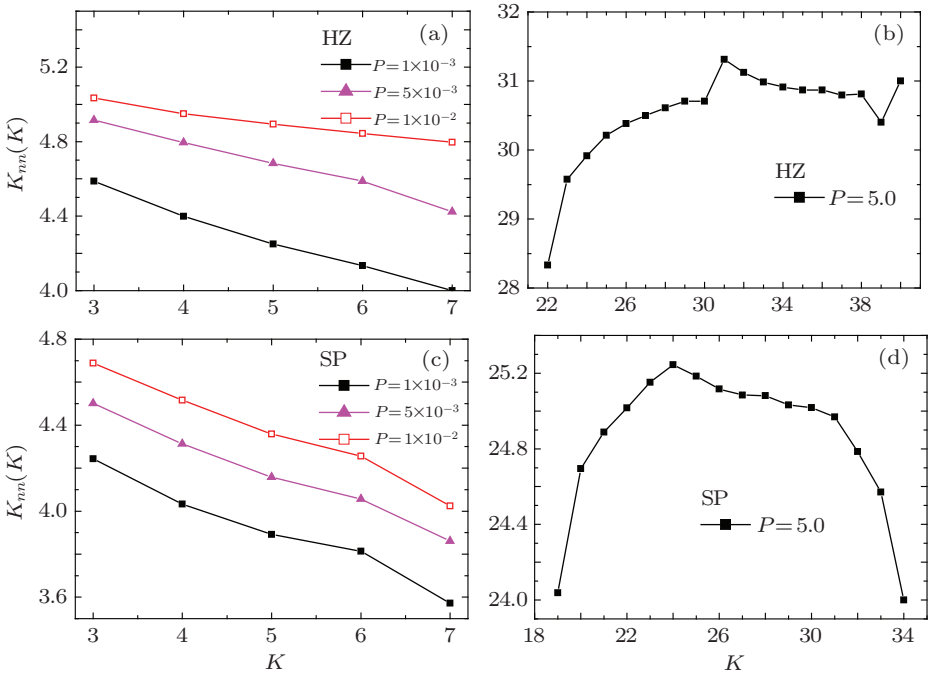


Fig. 6. (color online) $K_{nn}(K)$ of typical Hertzian (HZ) and harmonic (SP) systems. Panels (a) and (c): a marginally jammed system, (b) and (d): a deeply jammed system.

3.4. Cluster coefficient

Another fundamental quantity of a network is the clustering coefficient. It measures the number of triangle motifs in the system. A high value of clustering coefficient for an individual particle corresponds to a local close packed structure, whereas a low value means a locally loose packing. A triangular structure can reduce rotations and improve stability. Since a clustering coefficient is a measure of triangles, its drop corresponds to a loss of stabilizing structures in the material.[35]

Here we present the most standard and simplest clustering coefficient for the network.[27] The local clustering coefficient c_i of node i is first calculated, showing how likely two neighbors of node i are to be connected. The number of edges (e_i) in the subgraph G_i of i's neighborhood is firstly counted. Then c_i is the ratio between e_i and $k_i(k_i-1)/2$, the maximum possible number of edges in G_i:

$$c_i = \frac{2e_i}{k_i(k_i-1)} = \frac{\sum_{j,m} a_{ij} a_{jm} a_{mi}}{k_i(k_i-1)}. \tag{3}$$

The clustering coefficient of the graph is then given by the average of c_i over all the nodes: $C = N^{-1} \sum c_i$. By definition, $0 \leq c_i \leq 1$, and $0 \leq C \leq 1$. Figure 7 depicts the cluster coefficient for the Hertzian and harmonic systems at different pressures. One can see that C increases with pressure for both types of systems. In the marginally jammed region, C is a concave function, while in the deep jamming region, C is a convex function. This also shows that the deeply jammed solids have different structural properties from the marginally jammed solids. The transition pressure value (P_d) is slightly higher in the harmonic system because the harmonic contact is harder so that the system needs a higher pressure to enter the deep jamming region.

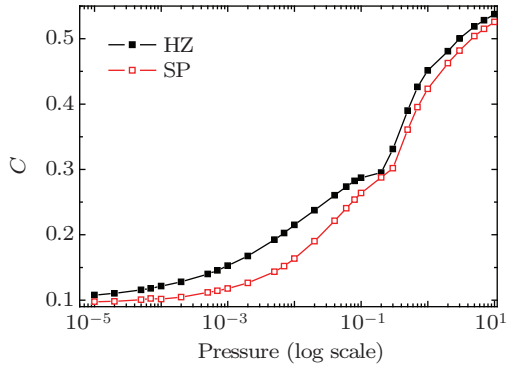


Fig. 7. (color online) Cluster coefficient for Hertzian and harmonic systems at different pressures.

4. Summary

In summary, we reported on some typical topological properties of contact force networks in marginally and deeply jammed granular packings based on the complex network theory. For both harmonic and Hertzian systems, the degree distribution, strength distribution, and degree correlation show remarkably different behaviors for the two types of jammed solids. In particular, the big and small particles show different correlation behaviors in the deep jamming state by using this simple packing system. The cluster coefficient also changes from a concave function to a convex function. All these differences prove that the two jamming states have very different network properties and this can lead to complex behavior in their dynamical performances.

The findings discussed here might be valuable in the perspective of complex spatial (or social) networks. While the marginally jammed system can represent the networks with nodes (persons) interacting only with their spatially nearest neighbors, the deeply jammed system can represent networks with nodes (persons) interacting with their spatially nearest neighbors and next nearest neighbors. The properties of deeply jammed solids reported here might reflect some behavior of these spatial (social) networks under some kind of external (social) pressure.

References

[1] Majmudar T S and Behringer R P 2005 *Nature* **435** 1079
[2] Shinbrot T and Muzzio F J 2001 *Nature* **410** 251
[3] Yan X, Shi Q, Hou M, Lu K and Chan C 2003 *Phys. Rev. Lett.* **91** 014302
[4] Shi Q, Sun G, Hou M and Lu K 2007 *Phys. Rev. E* **75** 061302
[5] Jiang Z, Lu K, Hou M, Chen W and Chen X 2003 *Acta Phys. Sin.* **52** 2244 (in Chinese)
[6] Shah S H, Li Y C, Cui F F, Zhang Q and Hou M Y 2012 *Chin. Phys. B* **21** 014501
[7] Hou M, Tu H, Liu R, Li Y, Lu K, Lai P and Chan C 2008 *Phys. Rev. Lett.* **100** 068001
[8] Li Y, Zhang Z, Tu H, Liu R, Hu H and Hou M 2009 *Acta Phys. Sin.* **58** 5840 (in Chinese)
[9] Li Y, Liu R and Hou M 2012 *Phys. Rev. Lett.* **109** 198001
[10] Shah S H, Li Y C and Hou M Y 2010 *Chin. Phys. B* **19** 108203
[11] Li Y Y, Xia W, Zhou Z Y, He K J, Zhong W Z and Wu Y B 2010 *Chin. Phys. B* **19** 024601
[12] Qadir A, Shi Q F, Liang X W and Sun G 2010 *Chin. Phys. B* **19** 034601
[13] Chen W, Hou M, Jiang Z, Lu K and Lam L 2001 *Europhys. Lett.* **56** 536
[14] Huang D, G Sun, M Hou and Lu K 2006 *Aata Phys. Sin.* **55** 4754 (in Chinese)
[15] Liu R, Li Y and Hou M 2008 *Acta Phys. Sin.* **67** 4660 (in Chinese)
[16] Cai Q D, Chen S Y and Sheng X W 2011 *Chin. Phys. B* **20** 024502
[17] Liu A J and Nagel S R 1998 *Nature* **396** 21
[18] Bi D, Zhang J, Chakraborty B and Behringer R P 2011 *Nature* **480** 355
[19] Xu N 2011 *Front. Phys. China* **6** 109
[20] O'Hern C S, Langer S A, Liu A J and Nagel S R 2002 *Phys. Rev. Lett.* **88** 075507
[21] O'Hern C S, Silbert L E, Liu A J and Nagel S R 2003 *Phys. Rev. E* **68** 011306
[22] Xu N, Wyart M, Liu A J and Nagel S R 2007 *Phys. Rev. Lett.* **98** 175502
[23] Xu N, Vitelli V, Wyart M, Liu A J and Nagel S R 2009 *Phys. Rev. Lett.* **102** 038001
[24] Xu N, Haxton T K, Liu A J and Nagel S R 2009 *Phys. Rev. Lett.* **103** 245701
[25] Zhang Z, Xu N, Chen D T N, *et al*. 2009 *Nature* **459** 230
[26] Zhao C, Tian K and Xu N 2011 *Phys. Rev. Lett.* **106** 125503
[27] Watts D J and Strogaz S H 1998 *Nature* **393** 440
[28] Barabási A L and Albert R 1999 *Science* **286** 509
[29] Boccaletti S, Latora V, Moreno Y, *et al*. 2006 *Phys. Rep.* **424** 175
[30] Barthelemy M 2011 *Phys. Rep.* **499** 1
[31] Arévalo R, Zuriguel I and Maza D 2009 *Int. J. Bifur. Chaos* **19** 695
[32] Ben-Nun O, Einav I and Tordesillas A 2010 *Phys. Rev. Lett.* **104** 108001
[33] Walker D M and Tordesillas A 2010 *Int. J. Solids Struct.* **47** 624
[34] Tordesillas A, Walker D M and Lin Q 2010 *Phys. Rev. E* **81** 011302
[35] Walker D M and Tordesillas A 2012 *Phys. Rev. E* **85** 011304
[36] Andrade J S, Herrmann H J, Andrade R F S and da Silva L R 2005 *Phys. Rev. Lett.* **94** 018702
[37] Johnson K L 1985 *Contact Mechanics* (Cambridge: Cambridge University Press)
[38] http://www.ece.northwestern.edu/∼nocedal/lbfgs.html.