Force percolation transition of jammed granular systems

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The mechanical and transport properties of jammed materials originate from an underlying percolating network of contact forces between the grains. Using extensive simulations we investigate the force-percolation transition of this network, where two particles are considered as linked if their interparticle force overcomes a threshold. We show that this transition belongs to the random percolation universality class, thus ruling out the existence of long-range correlations between the forces. Through a combined size and pressure scaling for the percolative quantities, we show that the continuous force percolation transition evolves into the discontinuous jamming transition in the zero pressure limit, as the size of the critical region scales with the pressure.

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I. INTRODUCTION

Amorphous particulate systems such as foams and granular materials jam and acquire mechanical rigidity when subjected to an external pressure [1–5]. In the jammed state, a network of interparticle forces determines resistance to shear [6,7], sound and heat transport [8–11], as well as electrical conductivity [12]. The distribution of the magnitude of the interparticle forces has been the subject of numerous studies [13–23], and it is now ascertained that this decays exponentially at large forces, while exhibiting a pressure dependent power law behavior at small forces. Large forces organize along chains [24–29], which suggests the existence of a large scale structure one might identify through statistical physics or network–based tools [30–37]. In this line of research, the main open question concerns the spatial organization of the force network, and the possible existence of long range correlations between the forces. These issues are conveniently investigated studying a force based bond percolation transition in which two particles are assumed to belong to a cluster if the magnitude of their interparticle force is larger than a threshold f_t (see Fig. 1). In the jammed phase, when $f_t = 0$ all contacting particles belong to the same cluster, while conversely in the $f_t \to \infty$ limit there are no clusters. Thus, a percolation transition occurs when the threshold overcomes a critical value f_c. Ostojic *et al.* [38] numerically investigated this force percolation transition in frictionless and frictional systems of disks packings prepared at constant pressure, finding a universal critical behavior and exponents not compatible with those of the random universality class. A recent experimental and numerical investigation of the force percolation transition of jammed disks packings at constant density [39] found different critical exponents, also not compatible with the random universality class. These results point towards the existence of long-range correlations between the forces. However, direct numerical and experimental investigations of the spatial correlation between the forces [15,40] failed to observe long correlation lengths. Accordingly, it is currently unclear whether the correlations between the forces of jammed packings are truly long ranged. The answer to this question might depend on the pressure/density of the system, that controls the percolation threshold f_c, as this must vanish at the jamming transition, as illustrated in Fig. 1, where all forces vanish. Thus, it is important to understand how the continuous force percolation transition in the zero pressure limit relates to the discontinuous jamming transition.

In this paper, we investigate force correlations in jammed granular packings via the numerical study of the force percolation transition of Harmonic and Hertzian particles, in both two and three spatial dimensions. First, we show that the force percolation transition does actually belong to the random universality class, regardless of the distance from the jamming threshold, thus ruling out the presence of long-range force correlations. Then we clarify how the features of the force

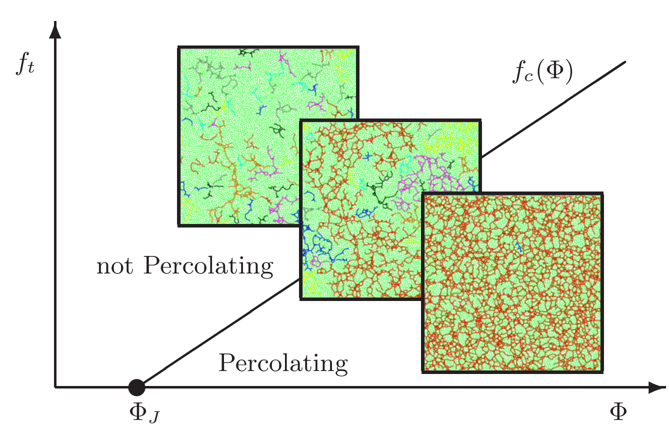

FIG. 1. A percolative analysis of jammed configurations is introduced by considering particles as connected if interacting with a force whose magnitude is greater than a threshold f_t. This schematic phase diagram illustrates the existence of a continuous percolation line that ends at the jamming volume fraction Φ_J, where the percolation transition becomes discontinuous. The panels illustrate the percolative analysis of a $N = 10^4$ particle system across the transition. Lines connect particles belonging to the same cluster. For clarity, not all of clusters are shown.

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percolation transition depend on pressure, thus rationalizing how the continuous force percolation transition evolves into the discontinuous jamming transition in the zero pressure limit.

II. MODEL AND SIMULATION DETAILS

We numerically [41] investigate systems of particles interacting via purely repulsive potential, $v(r) = \frac{1}{\alpha}\varepsilon(\frac{\sigma-r}{\sigma_1})^\alpha$ for $r < \sigma$, and $v(r) = 0$ for $r \geqslant \sigma$, where ε is the characteristic energy scale, σ is the average diameter of the interacting particles and r the distance between their centers. We study the system for two potentials, $\alpha = 2$ (harmonic) and $\alpha = 2.5$ (Hertzian), focusing on a 50:50 binary mixture of particles with diameters $\sigma_1 = 1$ and $\sigma_2 = \sigma_1/1.4$. We choose σ_1 and ε as our units of length and energy. We have considered various systems with number of particles from, $N = 10^3$ to $N = 8 \times 10^4$, at various values of the pressure p, from $p = 5 \times 10^{-6}$ to $p = 10^{-2}$. To prepare the system at the desired value of pressure, we first randomly distribute particles in a square or cubic box, with periodic boundary conditions. The size of the box is then repeatedly changed via a divide and conquer algorithm, where we minimize the elastic energy of the system using conjugate gradient algorithm after every change in simulation box size. This iterative procedure continues until the pressure equals the desired value with a tolerance of $|dp|/p < 10^{-6}$. For each dimensionality d, potential and pressure value, our results are averaged over 500 independent jammed configurations.

III. FORCE PERCOLATION

The force percolation transition is a bond percolation transition occurring on a disordered lattice whose nodes correspond to the particles, and whose bonds correspond to the interparticle forces. The percolation is induced by the removal of all bonds associated to interparticle forces f lower than the threshold force f_t, as the threshold f_t is varied. At each value of the pressure ($p > 0$) a percolation transition occurs as f_t varies, as schematically illustrated in Fig. 1. The percolative properties of this transition reflect those of the forces because the bonds that are retained are not randomly chosen, but correspond to interparticle forces greater than f_t.

We have determined the critical exponents governing the critical behavior of the strength of the percolating cluster P_∞, of the mean cluster size S, and of the percolation correlation length ξ, $P_\infty \sim |f - f_c|^\beta$, $S \sim |f - f_c|^{-\gamma}$, $\xi \sim |f - f_c|^{-\nu}$, performing a scaling analysis. Indeed, for finite systems the above critical behaviors are replaced by crossovers satisfying the scaling relations

$$P_\infty(N,f) = N^{-\frac{\beta}{d\nu}} m_1\big[N^{\frac{1}{d\nu}}(f - f_c)\big],$$
$$S(N,f) = N^{\frac{\gamma}{d\nu}} m_2\big[N^{\frac{1}{d\nu}}(f - f_c)\big], \quad (1)$$

with m_1 and m_2 universal scaling functions. If the considered system has a finite correlation length, then these scaling relations are valid as long as this length is smaller than the system size, $L \propto N^{1/d}$. To improve numerical accuracy we have performed a size scaling analysis of the fraction of particles in largest cluster C_1, that scales as P_∞ but is of easier investigation as it does not depend on the percolation threshold. The mean cluster size is defined as $S = \sum s^2 n(s)/\sum s n(s)$,

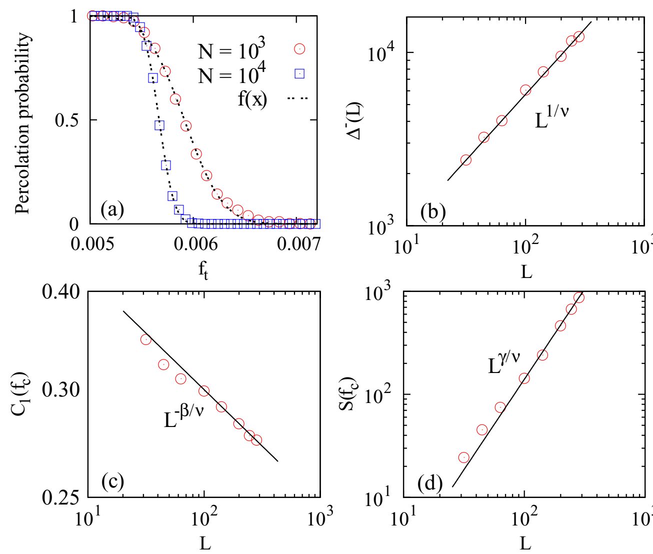

FIG. 2. Critical exponents of the force percolation transition: (a) Percolation probability as a function of force threshold f_t, fitted to sigmoidal function $f(x)$ (see text), (b) Inverse percolation transition width $\Delta^{-1}(L)$ scales as $L^{1/\nu}$, [(c) and (d)] largest cluster size C_1 and mean cluster size S at critical transition f_c scale as $L^{-\beta/\nu}$ and $L^{\gamma/\nu}$, respectively. Performing linear fits for the largest system sizes ($L > 100$), we estimate $\nu = 1.32(2)$, $\beta = 0.147(7)$, and $\gamma = 2.32(6)$. Data are for $p = 5 \times 10^{-3}$.

where s and $n(s)$ refer to the size and number of clusters, and the summation excludes the percolating cluster. The size s of a cluster equals its number of bonds.

IV. SIMULATION RESULTS

In this section, we present the results obtained by the numerical simulation of our model. Figure 2 illustrates the determination of the critical exponents of the force percolation transition for a two dimensional system of harmonic disks at pressure $p = 5 \times 10^{-3}$, we have conducted along the lines of Ref. [42]. This investigation strongly suggests the percolation transition to belong to the random percolation universality class. We first calculate the percolation probability, defined as the fraction of realizations with a system spanning cluster, as a function of threshold f_t for various system sizes L, which is a sigmoidal curve as shown in Fig. 2(a). This curve is then fitted to $f(x) = [1 - \text{erf}([f_t - f_c^e(L)]/\Delta L)]/2$, to obtain the effective percolation threshold $f_c^e(L)$ and the width of the percolation transition ΔL. From the expected size dependence of ΔL, $\Delta L \sim L^{-1/\nu}$, we estimate the critical exponent ν; result of Fig. 2(b) suggests $\nu = 1.32(2)$. Given the value of ν, we estimate the critical threshold considering that $f_c^e(L) - f_c \sim L^{-1/\nu}$, finding $f_c = 0.00549(5)$. Using f_c, the other two exponents are obtained using the scaling relations $C_1(f_c) \sim L^{-\beta/\nu}$ and $S(f_c) \sim L^{\gamma/\nu}$, yielding $\beta/\nu = 0.112(5)$ and $\gamma/\nu = 1.76(4)$, as shown in Figs. 2(c) and 2(d) respectively. Using the optimal value of $\nu = 1.32$, this gives $\beta = 0.147(7)$ and $\gamma = 2.32(6)$. We notice that these exponent values have been obtained through linear fitting procedures of the data of Fig. 2 corresponding to large system sizes, $L > 100$, as only for large systems the results becomes L independent.

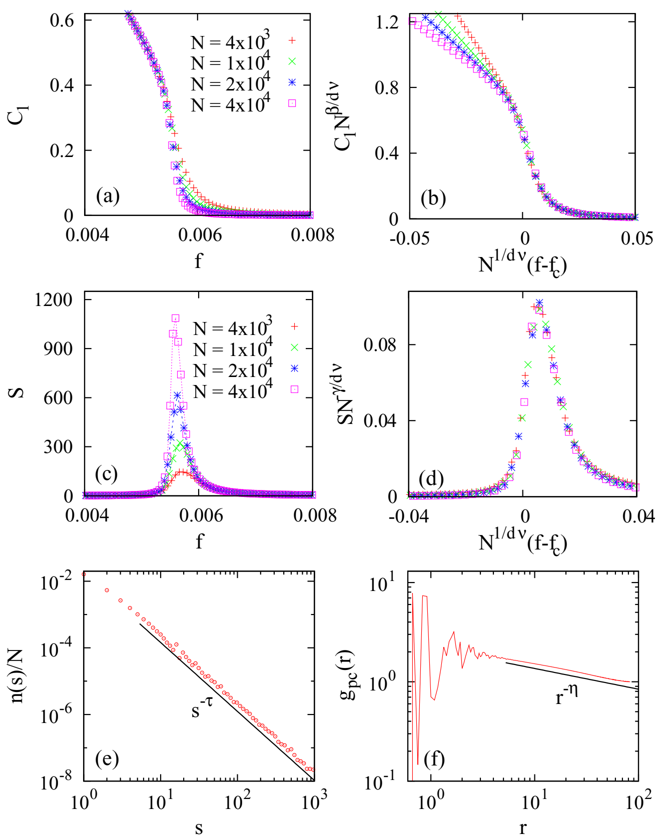

FIG. 3. Random percolation universality class of force percolation transition. Panels (a)–(d) show the finite-size scaling of the fraction of particles in the largest cluster C_1 and mean cluster size S using Eq. (1), and exponents determined in Fig. 2. Panels (e) and (f) show the normalized cluster size distribution $n(s)$, and the pair connected correlation function $g_{\rm pc}(r)$, respectively, at the percolation threshold for the $N = 4 \times 10^4$ system. Exponents are determined to be $\tau = 2.07(4)$, and $\eta = 0.208(6)$. Data are for $p = 5 \times 10^{-3}$.

This indicates, as discussed later on, the presence of a finite correlation length in our system. As a further validation of these findings, we show in Figs. 3(a)–3(d) that the data for C_1 and S collapse very well when scaled according to Eq. (1), for large system sizes. Additionally, Figs. 3(e) and 3(f) show the normalized cluster size distribution $n(s)$ and the radial distribution function of particles belonging to the percolating cluster $g_{\rm pc}(r)$ respectively, at the percolation threshold for the $N = 4 \times 10^4$ system. The distribution $n(s)$ fits well to the power-law decay $n(s) \sim s^{-\tau}$, with $\tau = 2.07(4)$. Similarly, for large r the pair-connected correlation function is well described by a power-law decay $g_{\rm pc}(r) \sim r^{-d+2-\eta}$, with $\eta = 0.208(6)$. We note that the exponent values we obtain match very well with the two-dimensional random percolation universality class exponents, $\nu = 4/3$, $\beta = 5/36$, $\gamma = 43/18$, $\tau = 187/91$, and $\eta = 5/24$ [43]. We have repeated this analysis for all values of the pressure we have considered, always finding values of the critical exponents compatible with those of the random universality class. In addition, analogous findings occur for the Hertzian potential, and in three dimensions, as we illustrate later in this paper. Summarizing, these results clarify that the force percolation transition is a continuous percolation transition in the random percolation universality class. As a consequence, the correlations between the interparticle forces of jammed packings are finite ranged.

It is worth noticing that these results contrast with those of Refs. [38,39], which suggested long-range correlations between the interparticle forces. First, Ref. [38] reported two exponents, $\phi = \frac{\gamma}{d\nu} = 0.89 \pm 0.01$, and $\nu = 1.6 \pm 0.1$. Of the two exponents, ϕ is compatible with the random percolation expectation, $43/48 = 0.895$, while ν, which is estimated with lesser accuracy, is not compatible with the random value, $\nu = 4/3$. We speculate that the difference is due to numerical errors arising from using small system sizes, as pointed in Ref. [39]. We notice that our exponent values, which are consistent with those of the random percolation transition in two dimensions, have been obtained through a linear fit procedure of the data shown in Fig. 2 corresponding to system sizes larger than $L > 100$, and that different values are obtained if all system sizes are considered. Second, Ref. [39] reported $\phi = 0.77$–0.85, and $\nu = 1.04$–1.58 depending on the packing fraction and polydispersity. Our speculation is that the differences from the random percolation values are due to using volume fraction as control parameter. For a fixed value of the volume fraction, in finite-size systems there are large fluctuations in the pressure values, and hence in the values of the critical threshold. When averaged over systems with different percolation thresholds, percolative quantities are expected to exhibit an effective critical-like behavior, the details depending on the distribution of the critical thresholds. Also, it is possible that the differences are due to different protocols used to prepare the jammed packings.

We now consider how the force percolation transition, that occurs at fixed pressure as the threshold force f_t varies, is related to the geometrically discontinuous jamming transition that occurs at $f_t = 0$, as the pressure/density varies. First, we note that the critical threshold f_c decreases with the pressure as $f_c \sim p^q$, with $q \approx 0.98$, as illustrated in Fig. 4. This is the same scaling we observe for the average force, that is commonly used [44] to decompose the force network in subnetworks with different mechanical properties. Next, in Fig. 5, we show the pressure dependence of cluster statistics.

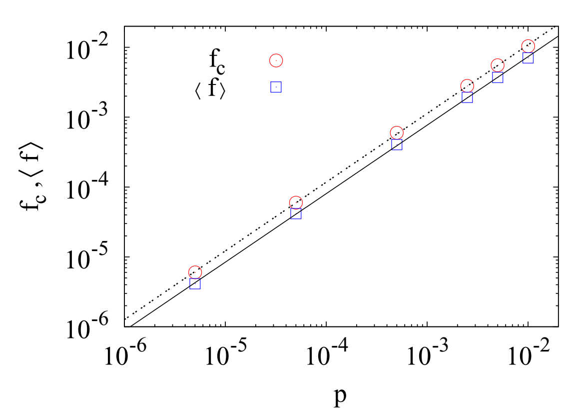

FIG. 4. Pressure dependence of the force percolation threshold, f_c, and of the average force, $\langle f \rangle$. These two forces are proportional, and scale as $f_c = \alpha_c p^q$ and as $\langle f \rangle = \alpha p^q$, with $q \approx 0.98(1)$, $\alpha_c = 1.00(4)$, and $\alpha = 0.67(3)$.

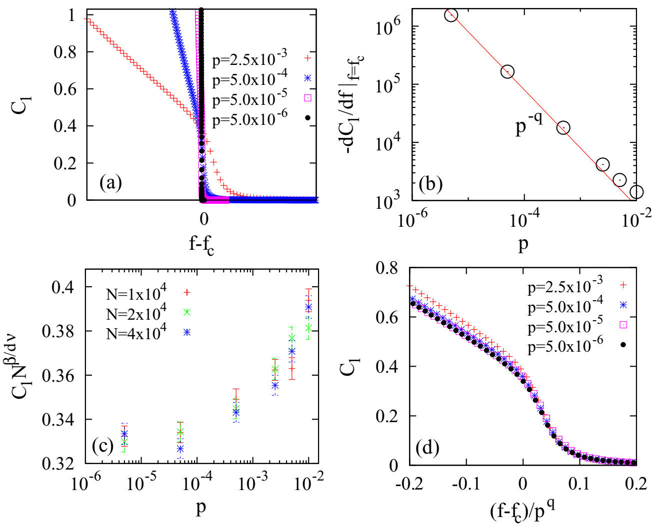

FIG. 5. Dependence of the size of the largest cluster, C_1, on $f - f_c$, for different values of pressure (a), and pressure dependence of its derivative at the inflection point (b). The derivative diverges as p^{-q} in the $p \to 0$ limit. Panel (c) clarifies that C_1 scales as $N^{-\beta/d\nu}$, for all values of the pressure, ruling out the presence of a discontinuous transition in the thermodynamic limit, for $p \to 0$. Panel (d) shows that the C_1 data of (a) collapse when plotted versus $(f - f_c)/p^q$, thus clarifying that the size of the critical region scales as p^q. In panels (a), (b), and (d), $N = 2 \times 10^4$.

We observe in Fig. 5(a) that the size of the largest cluster as function of the distance from the percolation threshold $f - f_c$ is pressure dependent, and becomes more abrupt when approaching the zero pressure limit. This tendency is quantified by investigating the derivative of C_1 at the inflection point, $dC_1/df|_{f=f_c}$. Figure 5(b) shows that this derivative increases in modulus as the pressure decreases, diverging as a power law $\sim p^{-k}$, with $k \simeq q$, in the zero pressure limit. This might suggest that the transition becomes discontinuous in the zero pressure limit. However, we show in Fig. 5(c) that C_1 at the inflection point has weak dependence on pressure, and that it scales as $N^{-\frac{\beta}{d\nu}}$ in the zero pressure limit $p \to 0$. Thus, C_1 does not exhibit a jump of finite size in the $p \to 0$ limit. These results suggest that in the zero pressure limit the force percolation transition remains a continuous transition, the only effect of the pressure being that of controlling the size of the critical region, which is expected to scale as p^q. We confirm this speculation in Fig. 5(d), where we illustrate that the data of panel a collapse when plotted as a function of $(f - f_c)/p^q$. Overall, these results suggest a combined size and pressure scaling for the strength of the percolating cluster, and, similarly, for the mean cluster size,

$$P_\infty(N,p,f) = N^{-\frac{\beta}{d\nu}} m_1\left[N^{\frac{1}{d\nu}} p^{-q}(f - f_c)\right],$$
$$S(N,p,f) = N^{\frac{\gamma}{d\nu}} m_2\left[N^{\frac{1}{d\nu}} p^{-q}(f - f_c)\right], \qquad (2)$$

where the exponent q is that controlling the dependence of the critical threshold on the pressure (see Fig. 4). The validity of the proposed scaling relations is confirmed by the good data collapse obtained for various pressure and system size, as shown in Fig. 6. Equation (2), and the scaling

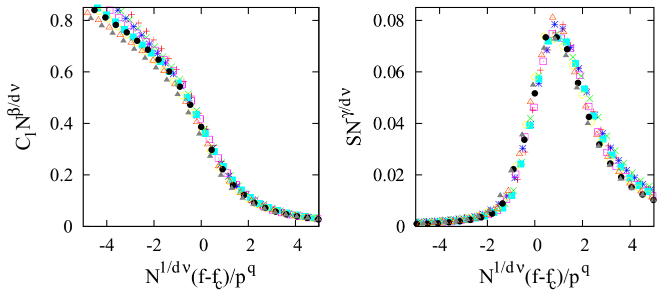

FIG. 6. Combined pressure and size scaling of the largest cluster size C_1 (left panel) and of the mean cluster size S (right panel). The presented data are for three system size $N = 4 \times 10^3$, 1×10^4, and 2×10^4, each corresponding to three pressure values $p = 5 \times 10^{-4}$, 5×10^{-5}, and 5×10^{-6}. We have fix $q \simeq 0.98$.

of the percolation threshold on the pressure, Fig. 4, clarify that the correlation percolation length, which measures the typical size of the cluster of forces larger than f, scales as $\xi = l[p^{-q}(f - f_c)]^{-\nu} = l(\alpha f/\langle f\rangle - \alpha_c)^{-\nu}$, with l pressure independent length scale. Since in the $p \to 0$ limit the force percolation transition does not become discontinuous, we understand that the order of the limits $p \to 0$ and $f \to 0$ matters. If the $p \to 0$ limit is carried out first, then the continuous force percolation transition is observed at $f = 0$. Conversely, if the $f \to 0$ limit is carried out first, then one observes the jamming transition at $f = 0$.

While these results show that there are no long-range force correlations, forces have short range correlations as revealed by the common observation of force chains. The presence of this length explains why we found critical exponents compatible with those of the random universality class only if we restrict our analysis to large systems, as in Fig. 2. Alternatively, short-range correlations can be revealed comparing the actual percolation threshold $f_c(p)$ to that obtained after removing all correlations, $f_c^R(p)$. The relation between $f_c^R(p)$ and $f_c(p)$ depends on the short-range correlation length, as well as on

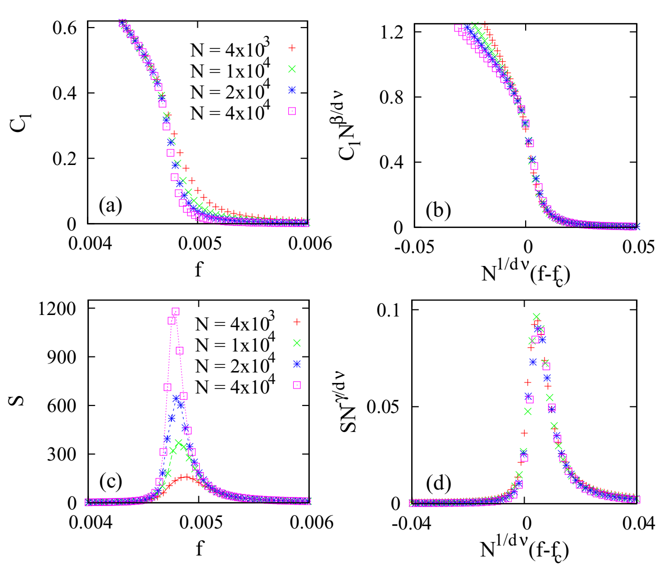

FIG. 7. Same as Fig. 3, but for Hertzian potential ($\alpha = 2.5$). The value of the pressure is $p = 0.005$.

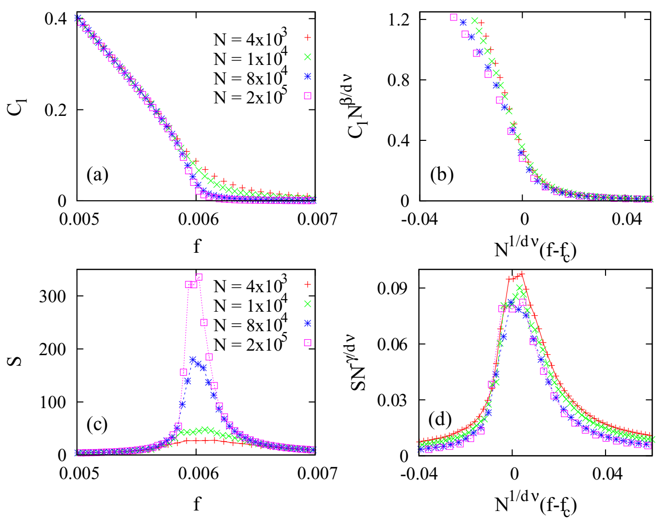

FIG. 8. Same as Fig. 3, for a system of Harmonic spheres in three dimensions. The value of the pressure is $p = 0.005$.

anisotropy of the correlations [45–48]. We have performed this investigation removing the force correlations by randomly swapping the forces associated to the different contacts, treating them as labels, and have found $f_c^R(p) < f_c(p)$. Importantly, we have found $f_c^R(p)/f_c(p) \simeq 0.6$ regardless of the pressure, in the $p \to 0$ limit, consistently with our proposed scenario according to which the pressure only fixes the size of the critical region.

Effect of potential and dimensionality. The finite-size scaling results presented in Fig. 3 for two-dimensional harmonic system hold equally well when using Hertzian potential (Fig. 7) and for three dimensions (Fig. 8). For the three-dimensional system in Fig. 8, we use the $d = 3$ random percolation exponents, $\nu = 0.87619$, $\beta = 0.4181$, and $\gamma = 1.793$ [43]. We observe a good collapse for C_1, showing that the critical exponents ν and β match with the random percolation values. The scaling of the mean cluster size reveals that a good data collapse is only obtained for the two largest systems we have considered. This implies that for smaller N the linear size of the system, that scales as $N^{1/3}$, is comparable to the force correlation length. Overall, we conclude that the force percolation transition belongs to the random percolation universality class, independent of the interaction potential and dimensionality.

V. CONCLUSIONS

Our investigation strongly suggests that the force percolation transition of jammed granular packings belongs to the random percolation universality class, regardless of the spatial dimension and of the interaction potential. The distance from the jamming threshold, that is fixed by the pressure of the system, controls the width of the critical region, that vanishes in the jamming zero-pressure limit. The main consequence of our findings is the absence of long-ranged correlations between the magnitudes of the forces in jammed granular packings. This result contrasts with earlier studies [38,39] of the force percolation transition, but agrees with numerical and experimental investigations of the spatial correlation between the forces [15,40]. It would be certainly of interest to perform experiments on jammed particulate systems, such as granular materials or emulsions, to experimentally settle this issue. In this respect, we stress that the random percolation scenario should be observed in experiments carried out at fixed pressure, rather than at constant volume fraction, as jammed systems at constant volume fraction exhibit very large pressure fluctuations. If the volume is fixed, the random percolation scenario is expected to emerge only for very large system sizes. It could also be possible that the observed correlations depend on the specific protocol used to prepare the jammed packings, that is known to affect the jamming density [49,50]. This is certainly an interesting future avenue of research.

Our work is also expected to help understanding the relation between the macroscopic properties of jammed systems and their structure. Indeed, forces in granular packings influence the nonaffine particle displacement resulting from externally imposed external deformations, which greatly affects the elastic response. In turn, this might allow connecting the percolation correlation length to other lengths that are known to characterize the elastic response of jammed systems [51–53]. In this line of research, we remark that recent results [54] have shown the existence of a point-to-set force correlation length that diverges at jamming, whose connection with the length scales characterizing the elastic response is also unclear.

As a final remark we notice that while in soft-sphere systems the jamming transition is investigated from above, $\phi > \phi_J$, in hard sphere systems one investigates it from below, $\phi < \phi_J$, jamming occurring at the volume fraction at which the pressure diverges when compressing the system. Below jamming, interparticle forces can be defined from the collisional momentum exchange [55]. While the features of the probability distribution of these forces has attracted much interest [56–60], little is known about their spatial correlation, which would be interesting to investigate using the force percolation approach.

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