Vibrations and Diverging Length Scales Near the Unjamming Transition

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We numerically study the vibrations of jammed packings of particles interacting with finite-range, repulsive potentials at zero temperature. As the packing fraction ϕ is lowered towards the onset of unjamming at ϕ_c, the density of vibrational states approaches a nonzero value in the limit of zero frequency. For $\phi > \phi_c$, there is a crossover frequency, ω^* below which the density of states drops towards zero. This crossover frequency obeys power-law scaling with ϕ-ϕ_c. Characteristic length scales, determined from the dominant wave vector contributing to the eigenmode at ω^*, diverge as power laws at the unjamming transition.

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The transition in which a disordered material becomes rigid encompasses a wide range of phenomena, from the liquid-glass transition to the onset of flow in granular materials or colloidal dispersions. There has been increasing convergence to the view that the onset of rigidity, or jamming, in a granular material and the onset of glassiness in a molecular liquid share many features in common [1–3]. An understanding of the origin of these commonalities may shed light on describing problems as diverse as force propagation through amorphous packings [4], dynamical heterogeneities in supercooled liquids [5], and the nature of the low-lying energy states of glasses [6,7].

In granular materials, which are effectively at zero temperature, a key parameter is the packing fraction of particles, ϕ. At a threshold packing fraction, ϕ_c, a granular material becomes mechanically stable—it jams. Studies of an idealized granular packing show that the jamming-unjamming transition has a mixed first-order–second-order character [8,9]. As such a system unjams with decreasing packing fraction, the number of interacting neighbors per particle drops discontinuously to zero. Despite this characteristic signature of first-order behavior, power-law scaling is also observed for other quantities [8]. This raises the question of whether there is a diverging length scale associated with the loss of rigidity. Simulations suggest that a diverging length scale exists on the low-density side of the transition [9,10], but there has been no demonstration of similar behavior in the jammed phase. Here we show that a diverging length can be extracted from the vibrational properties of the jammed phase.

In most crystalline or amorphous solids, vibrations at low frequency, ω, are expected to be long-wavelength, acoustic plane waves. From this assumption one obtains the asymptotic low-frequency Debye density of vibrational states: $\mathcal{D}(\omega) \propto \omega^{D-1}$ where D is the dimension of space. In this Letter, we conduct a systematic study of vibrational properties of frictionless, granular packings for volume fractions above the jamming transition. We find excess low-frequency modes that extend down to a characteristic frequency ω^*, below which $\mathcal{D}(\omega)$ drops towards zero. The crossover frequency ω^*, vanishes as a power law as ϕ approaches ϕ_c^+. Thus, ϕ_c marks the disappearance of a very unusual solid. Moreover, given ω^*, we can define a corresponding length scale, ξ, that diverges as a power law in ϕ-ϕ_c. Below ξ, the system behaves like the marginal solid at ϕ_c, while above ξ it behaves like an ordinary elastic solid [11].

The excess low-frequency vibrations that we find in our amorphous packings are reminiscent of phonon spectra in glasses [7]. Simulation studies of the Lennard-Jones glass found an excess of low-frequency vibrational modes [12] that increased as the system was diluted in an *ad hoc* fashion [13]. In another line of work, similar behavior is observed in fractal aggregates [14,15] as the particle density is lowered towards the percolation threshold [16]. By contrast, our system is not fractal even at the transition. Random networks also exhibit similar features [17]. Experiments on glassy systems show that there is a peak in $\mathcal{D}(\omega)/\omega^2$, known as the boson peak, that can increase in height and shift to lower frequency as the glass transition is approached [18]. The system we describe below allows us to observe an enhancement in low-frequency modes as we approach an unusual critical point.

In the simulations reported here we have studied monodisperse, soft spheres of diameter σ interacting through a finite-range, purely repulsive, harmonic potential:

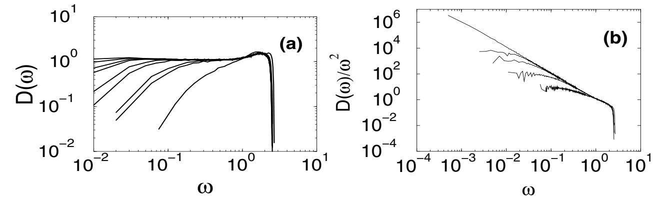

FIG. 1. (a) Density of vibrational states $\mathcal{D}(\omega)$, for $N = 1024$ monodisperse spheres, interacting via harmonic repulsions. The curves from right to left are for $\phi - \phi_c = 1 \times 10^{-1}$, 1×10^{-2}, 5×10^{-3}, 1×10^{-3}, 5×10^{-4}, 1×10^{-4}, 5×10^{-5}, 1×10^{-6}, and 1×10^{-8}. (b) $\mathcal{D}(\omega)/\omega^2$ at $\phi - \phi_c = 1 \times 10^{-6}$, 1×10^{-4}, 1×10^{-3}, 1×10^{-2}, and 1×10^{-1}, using data from $N = 1024$, 4096, and 10 000. Error bars are represented by the scatter in the data.

$$V(r) = \begin{cases} V_0(1 - r/\sigma)^2 & r < \sigma \\ 0 & r \geq \sigma \end{cases}.$$

Here, r is the center-to-center separation between two particles. The units of length and time are σ and $(md^2/V_0)^{1/2}$, respectively, for particles of mass m. Our three dimensional ($3D$) systems consist of $1024 \leq N \leq 10000$ spheres in periodic cubic simulation cells. We employ a compression/expansion algorithm followed by conjugate-gradient energy minimization to obtain $T = 0$ configurations [8]. We also studied bidisperse, harmonic discs in $2D$, as well as Hertzian contact potentials in $3D$. Our conclusions are the same for all three systems.

Figure 1(a) shows the density of states (computed from the dynamical matrix [19]), $\mathcal{D}(\omega)$, as a function of ω covering eight decades in $(\phi - \phi_c)$, averaged over 10 configurations for $N = 1024$. For the smallest value of $(\phi - \phi_c)$, the low-frequency behavior approaches a flat spectrum with an intercept of $\mathcal{D}_0 \equiv \mathcal{D}(\omega \to 0)$. Similar behavior is seen in fractals [15] and random networks [17]. Thus, close to the jamming transition there is no longer any vestige of Debye behavior. As the system is compressed above threshold, the curves depart from this plateau behavior at a frequency ω^*, which increases with $(\phi - \phi_c)$. Below ω^*, $\mathcal{D}(\omega) \to 0$ as $\omega \to 0$. Experiments on vitreous silica [20] and simulations of glasses with three-body interactions [21] have observed a similar trend with decreasing pressure. Figure 1(b) shows $\mathcal{D}(\omega)/\omega^2$ for all N at several values of $(\phi - \phi_c)$. For $N > 1024$, data is averaged over 3–5 configurations. The peak position shifts to lower frequencies and the peak height increases as ϕ_c is approached, analogous to the way some glasses behave as the glass transition temperature is approached [18].

Figure 2 shows the crossover frequency ω^* versus $(\phi - \phi_c)$. We determine ω^* by finding where $\mathcal{D}(\omega)$ for a given $(\phi - \phi_c)$ departs from $\mathcal{D}(\omega)$ for the next smallest value of $(\phi - \phi_c)$. Over more than 4 decades in $(\phi - \phi_c)$:

$$\omega^* \propto (\phi - \phi_c)^{\Omega} \tag{1}$$

with $\Omega = 0.48 \pm 0.03$. The scaling is robust, independent

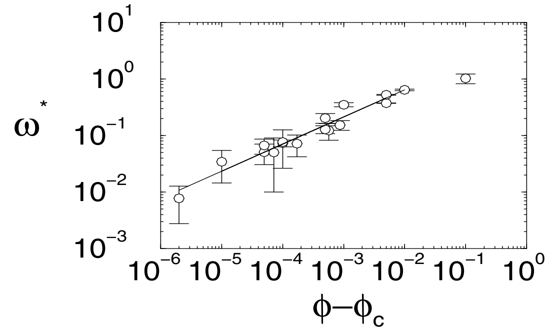

FIG. 2. The crossover frequency ω^*. The line is a fit to Eq. (1) with $\Omega = 0.48$.

of the precise manner in which we determine ω^*. It is the same (with different prefactors) when ω^* is defined as the value of ω at which $\mathcal{D}(\omega)$ reaches D_0, $0.9D_0$, or $0.5D_0$, as well as the frequency where $\mathcal{D}(\omega)/\omega^2$ in Fig. 1(b) levels off with decreasing ω.

Given ω^*, we define a corresponding length scale, ξ_T, that diverges as $\phi \to \phi_c^+$. To extract ξ_T, we examine the spatial variation of the eigenmode corresponding to the frequency ω^*. We take the Fourier transform of the appropriate component of the polarization vector $\mathbf{P}_i(\omega^*)$, of each particle i, which for transverse waves is [22],

$$f_T(k, \omega^*) = \left\langle \left| \sum_i \hat{\mathbf{k}} \wedge \mathbf{P}_i(\omega^*) \exp(i\mathbf{k} \cdot \mathbf{r}_i) \right|^2 \right\rangle,$$

where $\langle\rangle$ denotes an average over configurations and over all wave vectors with the same magnitude k. (The longitudinal component, $f_L(k, \omega)$, not shown, is the dynamical structure factor accessible from inelastic neutron scattering.) Fig. 3(a) shows these functions at the values of ω^* determined for different compressions, $(\phi - \phi_c)$. The transverse components exhibit well-defined peaks at small wave vectors k^* (there is a system size cutoff at $k_{\min} = 2\pi/L$, where L is the size of the simulation box). Thus, $\xi_T \equiv 2\pi/k^*$ is the dominant transverse length scale for that mode. Figure 3(b) shows ξ_T as a function of $(\phi - \phi_c)$. The solid line corresponds to a power-law fit:

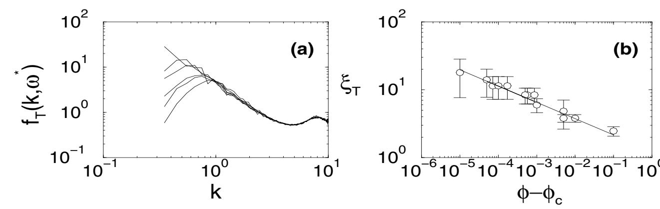

FIG. 3. (a) Transverse spectral functions $f_T(k, \omega^*)$ for $\phi - \phi_c = 1 \times 10^{-5}$, 5×10^{-5}, 1×10^{-4}, 5×10^{-4}, 1×10^{-3}, and 5×10^{-3}, with decreasing amplitude, respectively. (b) The correlation length $\xi_T \equiv 2\pi/k^*$ obtained from the wave vector k^* for the position of the peak in f_T at frequency ω^*. Data obtained from all system sizes.

$$\xi_T \propto (\phi - \phi_c)^{-\nu_T}, \tag{2}$$

with $\nu_T = 0.24 \pm 0.03$. The exponents ν_T and Ω [Eq. (1)] can be related to each other via a simple scaling argument using $k^* = \omega^*/c_T(\phi)$, where $c_T(\phi)$ is the velocity of transverse sound. The shear modulus G_∞ vanishes with an exponent of $\gamma = 0.48 \pm 0.05$ [9], implying that $c_T(\phi)$ vanishes with an exponent of 0.24. Given $\Omega = 0.48$, we would therefore expect $\nu_T = \Omega - \gamma/2 \approx 0.24$, in agreement with the results of Fig. 3(b).

A similar argument can be constructed for a longitudinal length ξ_L based on the peak of $f_L(k, \omega^*)$. Although it is difficult to extract the peak value from $f_L(k, \omega^*)$ because the peaks occur at very low values of k, the analogous scaling relation based on the longitudinal sound speed [and hence the bulk modulus, which is independent of $\phi - \phi_c$ [9]] predicts

$$\nu_L \approx 0.48. \tag{3}$$

We also simulated systems with Hertzian potentials: $V_0(1 - r/\sigma)^{5/2}$, for $r < \sigma$, and zero otherwise. In this case, we find that ω^* vanishes with an exponent $\Omega \approx 0.78 \pm 0.03$, which is different from that obtained for the harmonic case. However, by calculating the peak of $f_T(k, \omega^*)$ we obtain a length scale ξ_T that diverges with $\nu_T \approx 0.23$, just as in the harmonic case. This is consistent with the scaling argument based on the speed of sound, since the shear modulus vanishes with an exponent $\gamma \approx 0.95$ for the Hertzian case [9]. Thus, for the Hertzian and harmonic potentials, we have the same scaling for ξ_T, suggesting the transition is universal.

The strong departure from the low-frequency Debye density of states suggests that the eigenmodes are poorly characterized by simple plane waves [23]. We illustrate this point in Fig. 4 where we show the lowest frequency modes for 2D harmonic systems at the two extreme values of $(\phi - \phi_c) = 1 \times 10^{-1}$ and 1×10^{-8}. We show 2D results here for ease of visualization. These correspond to modes below and above ω^*, respectively, for those packing fractions. In the compressed system at $\omega < \omega^*$ the eigenmode

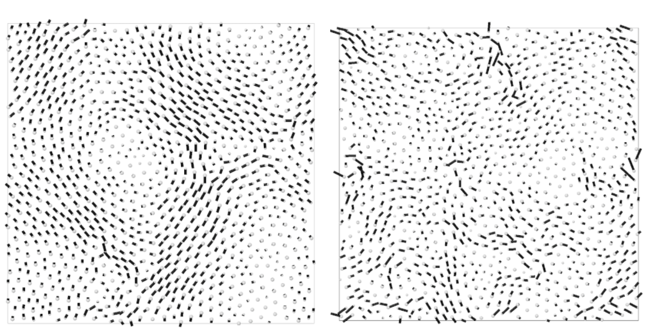

FIG. 4. Lowest frequency eigenmodes for $N = 1024$ bidisperse discs in 2D, at two extreme values of $\phi - \phi_c$: 1×10^{-1} (left), and 1×10^{-8} (right). The dots represent the centers of the particle and the black lines their polarization vectors.

retains identifiable correlated plane-wave-like character, consistent with the more Debye-like behavior of $\mathcal{D}(\omega)$ as $\omega \to 0$. In contrast, when $\omega > \omega^*$ as in the system closest to ϕ_c, all plane-wave character is lost. This picture suggests that ξ_T represents the length scale above which one can average over disorder: wave vectors of magnitude $k > 2\pi/\xi_T$ do not have long enough wavelengths for effective averaging to take place. This is related to the criterion that characterizes the elastic-granular crossover in a Lennard-Jones glass [24].

Our results for ω^* and ξ_T have motivated three theoretical papers that treat different aspects of the zero-temperature jamming transition. A soft-mode analysis by Wyart *et al.* [11] predicts a constant density of states in the isostatic limit [25] (achieved in our system at ϕ_c [8,9]). For $\phi > \phi_c$, they predict a crossover frequency ω^*, that vanishes with power laws that agree with our findings. They also identify a diverging length scale consistent with our prediction for ξ_L [Eq. (3)]. The approach by Schwarz *et al.* [26] relates jamming at ϕ_c to the onset of k-core percolation. For the Bethe lattice, they find a correlation length exponent of $\nu = 1/4$, in agreement with Eq. (2), as well as another length scale with $\nu^\# = 1/2$, in agreement with predictions of Wyart *et al.* [11] and our Eq. (3). Henkes *et al.* [27] proposed a field-theory of 2D packings and argued for two diverging length scales at the jamming transition in agreement with Eqs. (2) and (3). Finally, a diverging length scale was measured in simulations by Drocco *et al.* [10], on approach to the jamming threshold *from below.* This length scale exponent was found to be $\nu_- = 0.6$–0.7, in agreement with the finite-size scaling analysis of jamming thresholds [8,9].

Thus, four relevant length scales emerge in describing the jamming-unjamming transition: (i) The interparticle overlap distance, which goes linearly to zero at ϕ_c [9]. (ii) The length scale determined from finite-size scaling [8,9] and that obtained on the low-density side of the transition [10]. These diverge with an exponent ~ 0.7. (iii) The diverging length scale presented here on the high-density side of the transition, determined from transverse vibrations; this diverges with an exponent of 0.24. (iv) Theories [11,26] and a scaling argument based on our data [Eq. (3)] suggest a diverging length scale with exponent 0.5. It is still not clear how all these different length scales are tied together. That different exponents are observed on different sides of the transition suggests that the jammed phase may always be separated from the unjammed one by a singularity.

In conclusion, we have studied the properties of the jamming-unjamming transition at zero temperature. The loss of rigidity is characterized by a diverging length scale, and a discontinuity in the number of interacting neighbors [8,9]. This suggests that unjamming may be most properly described as a second-order transition with a universal jump in the order parameter.

Fractal objects can show anomalous scaling in the density of states with an excess of low-frequency modes [14–16]. In contrast, at the transition our system is already dense and thus more similar to that of a glass.

Our results suggest that the excess vibrations of glasses are a pale reflection of properties at the jamming transition: we see a density of states which can produce a boson peak that diverges at the transition, where the vanishing of the boson peak frequency is accompanied by a diverging length scale. We suggest that the excess density of states can be observed experimentally in dense colloidal suspensions and emulsions by measuring the trajectory of a few tracer particles. This would test the proposed connection between glasses and athermal systems near the jamming transition.

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