Universal Non-Debye Scaling in the Density of States of Amorphous Solids

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At the jamming transition, amorphous packings are known to display anomalous vibrational modes with a density of states (DOS) that remains constant at low frequency. The scaling of the DOS at higher packing fractions remains, however, unclear. One might expect to find a simple Debye scaling, but recent results from effective medium theory and the exact solution of mean-field models both predict an anomalous, non-Debye scaling. Being mean-field in nature, however, these solutions are only strictly valid in the limit of infinite spatial dimension, and it is unclear what value they have for finite-dimensional systems. Here, we study packings of soft spheres in dimensions 3 through 7 and find, away from jamming, a universal non-Debye scaling of the DOS that is consistent with the mean-field predictions. We also consider how the soft mode participation ratio evolves as dimension increases.

Introduction.—Although amorphous solids (such as foams, grain packings, and glasses) constitute most of solid matter, they are so poorly understood that many textbooks focus almost exclusively on their crystalline counterpart. However, thanks to an exact solution of a model for jamming and a complementary description of mechanical marginality [1,2], our fundamental understanding of these solids has recently exploded. Yet these advances also leave open many questions concerning their applicability to real systems, especially away from the jamming transition.

One such question is the microscopic origin of the boson peak, which is an excess of vibrational modes in the density of states (DOS) of amorphous solids with respect to Debye's standard model for phonons in crystalline solids [3]. Since the boson peak anomaly was carefully studied by Raman and neutron scattering [4–6], it has been given a variety of explanations, ranging from specific features of interatomic forces to a broadened van Hove singularity [7]. From the viewpoint of amorphous solids as the paragon of disorder, various models have also been advanced [8–11].

Here, we consider a proposal that recently emerged from the study of the simplest model of amorphous solids: a disordered assembly of soft, purely repulsive spheres at zero temperature under a confining pressure P. This jammed solid becomes mechanically unstable at a sharply defined jamming transition, upon reaching $P = 0$ [12]. The study of this transition by statistical and soft-matter physics [13] has revealed that the geometric [14], rheological [15], vibrational [16,17], and elastic properties [18] of solids close to jamming markedly differ from those of crystals.

In particular, precisely at the jamming transition the DOS $D(\omega)$, with frequency ω, becomes flat for $\omega \rightarrow 0$, which leads to a diverging boson peak [17,19]. It is thus natural to wonder what is the low-frequency behavior of $D(\omega)$ in the vicinity of this transition, and whether it could provide an explanation of the boson peak also away from this singular point.

A crucial concept associated with jamming is that of *marginal stability*. At the jamming transition the system is on the verge of mechanical instability, which naturally gives rise to low-energy excitations [17,18]. Surprisingly, it was recently shown that amorphous solids remain marginally stable even at finite pressures, and, by means of effective medium theory, that this marginality leads to a modified Debye behavior with $D(\omega) \sim \omega^2$—as in crystals but with a constant prefactor much larger than expected from standard elasticity [16,20]. This result offers a promising account for the boson peak. Interestingly, the same scaling behavior was also recently uncovered in the perceptron, which is an exactly solvable model in the same universality class as soft spheres close to jamming [21]. This concordance likely results from both effective medium theory and the perceptron being mean-field descriptions that are expected to exactly capture the behavior of infinite-dimensional systems [22].

Before considering possible shortcomings of such descriptions, let us first detail their predictions. Away from jamming, at large length scales a solid should behave as a continuous medium. One therefore expects a Debye scaling of the DOS at low frequency, i.e., $D(\omega) \sim \omega^{d-1}/c^d$, where c is the speed of sound in the solid. Upon approaching

jamming, the speed of sound of transverse (shear) waves vanishes as $c_T = \sqrt{G/\rho} \propto \sqrt{\omega_*}$, where ω_* is a characteristic frequency that vanishes at jamming, $G \propto \omega_*$ is the shear modulus, and ρ is the number density [12]. Close to jamming, transverse waves should thus dominate the low-frequency regime. Combining this result with marginal stability, effective medium theory [20] indeed gives

$$D(\omega) \sim \begin{cases} \omega^{d-1}/\omega_*^{d/2} & \omega \ll \omega_0 \\ \omega^2/\omega_*^2 & \omega_0 \ll \omega \ll \omega_* \\ \text{const} & \omega \gg \omega_* \end{cases} \quad (1)$$

where ω_0 is a threshold frequency that separates the Debye from the anomalous ω^2 regime. Interestingly, for infinite-dimensional, marginally stable systems, the exact solution of the perceptron shows that $\omega_0 = 0$ for a finite region around jamming [21], implying that the Debye regime disappears altogether. In $d = 3$, although both the Debye and the anomalous regimes scale as ω^2, the prefactor of the latter, $1/\omega_*^2$, diverges much faster than the Debye prefactor, $1/\omega_*^{3/2}$, upon approaching the jamming transition (as was numerically validated in Ref. [20]). Thus, even for $\omega_0 > 0$, the anomalous regime is expected to bury the Debye scaling in systems sufficiently close to jamming.

Further validating these predictions is, however, non-trivial. For obvious physical reasons, most studies of amorphous solids have explored the nature of excitations in two- or three-dimensional systems. These results, however, may be strongly influenced by low-dimensional effects that are absent from mean-field descriptions and may partially obfuscate the universality of the phenomenon. For instance, some of the low-frequency excitations are known to be spatially quasilocalized [23–25] and are associated with structural soft spots [26], while only purely delocalized modes can be found in infinite dimensions [21]. The finite-dimensional behavior of ω_0 may also be richer than in infinite-dimensional models. In this Letter, we reconcile physical systems and mean-field theories by studying the vibrational modes of soft-sphere packings both as a function of packing fraction and spatial dimension. In doing so, we disentangle universal from low-dimensional features of the vibrational spectrum, similarly to what has been done for the force network [27,28]. We remarkably find that the ω^2 regime is present in all dimensions down to the lowest numerically accessible frequencies.

Model description and Hessian.—We generate packings of N frictionless spheres (N ranges from 1024 to 16 384) interacting via a one-sided (contact) harmonic potential within a periodic cubic box in $d = 3$–7. The total system energy is $U = \frac{1}{2} \sum_{i<j}^{N} \Theta(\sigma - r_{ij})(\sigma - r_{ij})^2$, where σ is the particle diameter, r_{ij} is the distance between particles i and j, and Θ is the Heaviside step function. The relevant control

parameter is the packing fraction, $\phi = \rho V_d(\sigma)$, where $\rho \equiv N/V$ for a system of volume V and $V_d(\sigma)$ is the d-dimensional volume of a ball of radius σ. Initializing with Poisson-distributed spheres at very high ϕ, configurations are obtained by iteratively (i) deflating particles in small steps and (ii) minimizing the system energy, using the numerical scheme described in Refs. [28,29]. For $\phi > \phi_J$ we obtain jammed packings with locally minimal $U > 0$, while for $\phi < \phi_J$ configurations are unjammed, and hence not mechanically stable at $T = 0$. The limit case $\phi = \phi_J$ and $U = 0$ is the jamming transition for a given initial configuration. We thus define the excess packing fraction $\Delta\phi \equiv \phi - \phi_J$. (For this system pressure $P \propto \sqrt{U} \propto \Delta\phi$ [12,28].)

In order to extract information about the harmonic excitations of the system, we compute the Hessian matrix

$$H_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial r_i^\alpha \partial r_j^\beta} = \delta_{ij} \sum_{k \in \partial i} \left[n_{ik}^\alpha n_{ik}^\beta + \frac{\varepsilon_{ik}}{r_{ik}} (n_{ik}^\alpha n_{ik}^\beta - \delta^{\alpha\beta}) \right] - \delta_{\langle ij \rangle} \left[n_{ij}^\alpha n_{ij}^\beta + \frac{\varepsilon_{ij}}{r_{ij}} (n_{ij}^\alpha n_{ij}^\beta - \delta^{\alpha\beta}) \right],$$

where $\alpha, \beta = 1 \ldots d$ are vector components, $\varepsilon_{ij} = \sigma - r_{ij}$ is the overlap between two spheres, $n_{ij} = (\mathbf{r}_j - \mathbf{r}_i)/r_{ij}$ is a unit vector, both δ_{ij} and $\delta^{\alpha\beta}$ are Kronecker deltas, $\delta_{\langle ij \rangle}$ indicates a contact between a pair of particles, and ∂i denotes the set of neighbors of i. The eigenvectors $\{u_i^\alpha\}_k$ and eigenvalues λ_k of the Hessian then provide the vibrational modes and their angular frequencies, $\omega_k = \sqrt{\lambda_k}$, respectively.

Universal low-frequency scaling.—In all dimensions d studied, $D(\omega)$ is found to have the same overall shape, independently of system size. Figure 1 illustrates this
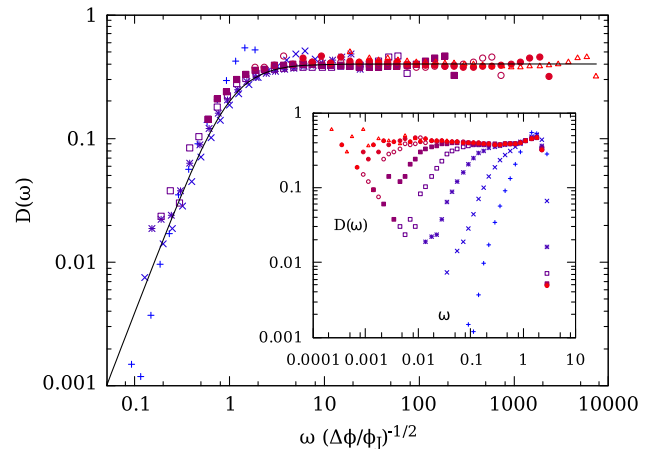

FIG. 1. DOS for a single configuration in $d = 4$ for $N = 8192$ with rescaled ω. The collapsed data are fitted to Eq. (3) (solid line). Inset: DOS for $\Delta\phi/\phi_J = 9.1 \times 10^{-8}$, 9.2×10^{-7}, 9.2×10^{-6}, 9.2×10^{-5}, 9.0×10^{-4}, 8.7×10^{-3}, 8.0×10^{-2}, and 9.4×10^{-1}, from left to right. Errors are smaller than the symbol size, except at very low ω, where they are comparable to the data scatter.

universality for $d = 4$. At $\Delta\phi = 0$, the nontrivial part of the DOS, i.e., excluding rattlers, goes to a constant for $\omega \to 0$, as has been widely reported in $d = 2$ and 3 [16–18]. For $\Delta\phi > 0$, the DOS peels off from the plateau below a given ω_*. It has been argued theoretically [16] and observed in $d = 3$ [17] that this crossover should scale as $\omega_* \propto \sqrt{\Delta\phi}$. Here also, this scaling collapses $D(\omega)$ onto a single master curve at small $\Delta\phi$ (Fig. 1).

From the rescaled results, we clearly see that below ω_* the DOS scales as ω^2 in all d, as in the mean-field descriptions [20,21]. In order to further scrutinize these results we use the perceptron DOS [21],

$$D(\omega) = \frac{\omega^2 (\omega_{max}^2 - \omega^2)^{1/2}/\pi}{\omega^2 + \omega_*^2}, \qquad (2)$$

where ω_{max} is the highest frequency. The model is not translationally invariant and thus its DOS never reaches a Debye-like regime, even as $\omega \ll \omega_0$, but as long as $\omega_0 \ll \omega \ll \omega_{max}$, we can reasonably fit the soft sphere results to a generalized form,

$$D(\omega, \Delta\phi) \approx \frac{A\omega^2}{\omega^2 + B\Delta\phi/\phi_J}, \qquad (3)$$

with free parameters A and B (Fig. 1). Remarkably, Eq. (3) captures the collapse of the DOS in all d, with roughly the same fitted values for $A \approx 0.4$ and $B \approx 1$ in all cases (Fig. 2, top). We thus consistently determine that ω_0 is smaller than the observable range of frequencies, which is compatible both with a very weak scaling of ω_0 with $\Delta\phi$ and its complete vanishing, as observed in infinite-dimensional models.

This scaling universality does not, however, extend to very large $\Delta\phi$. For $\Delta\phi/\phi_J \gtrsim 1$, the DOS systematically deviates from the master curve on which the lower packing fraction results effortlessly collapse (Fig. 2). The low frequency regime then grows faster than ω^2 in all dimensions, but is not Debye-like either. In fact, no clear power-law scaling can be observed. Interestingly, the results nonetheless tend toward a dimensionally independent form as d increases (Fig. 2, bottom), suggesting a certain universality. A possible interpretation is that the various scaling regimes are then mixed, with $\omega_0 \sim \omega_* \sim \omega_{max}$; hence, the phenomenological form [Eq. (3)] fails. The weak dimensional dependence might result from the integration within the force network—which occurs for $\Delta\phi \approx 0.1$—of particles that were rattlers at ϕ_J, whose density decays exponentially quickly with increasing d (Fig. 2, inset) [27]. Although we cannot provide a clear resolution of these effects here, we get back to this issue in the conclusion.

Localization.—In light of the remarkable agreement between the infinite-dimensional mean-field theory and numerical results for soft spheres (for $\Delta\phi/\phi_J \lesssim 1$), one may wonder if their eigenmode structure is also similar. In $d = 2$ and 3, however, soft spheres are known to have low-frequency modes that are quasilocalized [11,23,24,26], while modes in infinite dimensions are always perfectly
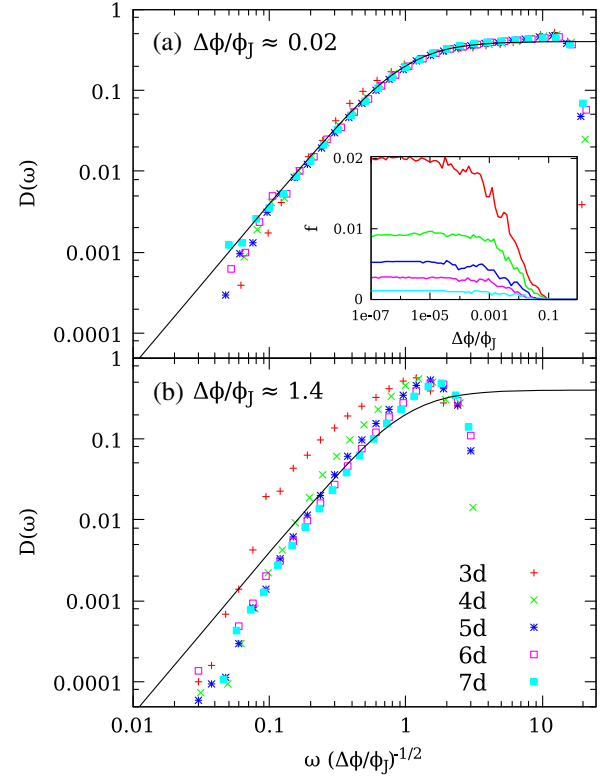

FIG. 2.   DOS for $N = 8192$ in $d = 3$ to 7 averaged over 30 to 50 configurations for (a) moderately compressed $\Delta\phi/\phi_J \approx 0.2$ and (b) highly compressed $\Delta\phi/\phi_J \approx 1.4$ above jamming. The solid line gives Eq. (3) with the fit parameters obtained in Fig. 1. Inset: the fraction f of rattlers in the system (and hence the fraction of trivial zero modes in the DOS) vanishes around $\Delta\phi \approx 0.1$, and is exponentially suppressed with dimension [27]. Errors are smaller than the symbol size, except at very low ω, where they are comparable to the data scatter.

delocalized [21], because particles then have an infinite number of neighbors and the model becomes effectively long range. To study the evolution of eigenmode localization with d, we assess the degree of localization of each eigenmode $\{ \mathbf{u}_i(\omega) \}$ by measuring its inverse participation ratio (IPR) [30],

$$Y(\omega) = \frac{\sum_i^N |\mathbf{u}_i(\omega)|^4}{[\sum_i |\mathbf{u}_i(\omega)|^2]^2}. \qquad (4)$$

By this measure, a mode that is completely localized on a single particle has $Y = 1$, while a mode extended over the full system has $Y \sim N^{-1}$.

Figure 3 shows the evolution of the IPR with frequency in $d = 4$ for different $\Delta\phi$. Following Ref. [24], we distinguish three regimes: (i) at low frequency, we find relatively localized modes with intermediate IPR (as in the Heisenberg model [30]); (ii) at intermediate frequency, we find a band of extended modes with $Y \sim 1/N$; and (iii) at high frequency, Y remains of order $1/N$ but with a quickly increasing prefactor, signalling incipient localization at the band edge. This categorization is also supported by the finite-size scaling
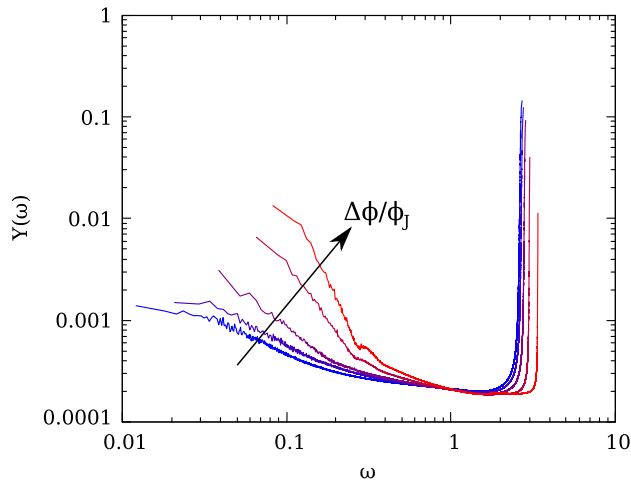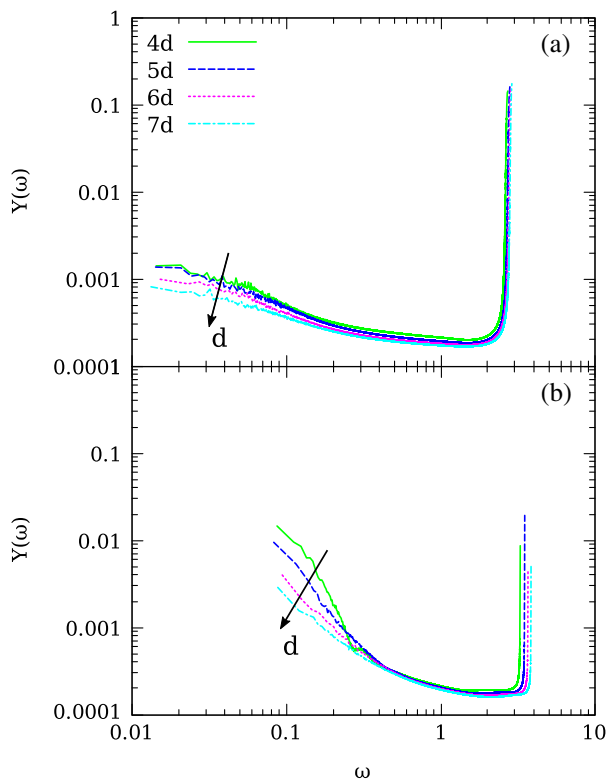
FIG. 3.   Evolution of IPR with frequency in $d = 4$ for $N = 8192$ averaged over 50 configurations for $\Delta\phi/\phi_J = 1.5 \times 10^{-2}$, 4.7×10^{-2}, 1.5×10^{-1}, 5.1×10^{-1} and 1.6. Statistical errors are comparable to the data scatter.

of the IPR [31]. In addition to its robust evolution with frequency, $Y(\omega)$ shows an interesting dependence on $\Delta\phi$ and d. As $\Delta\phi$ increases, low-frequency modes become increasingly localized (Fig. 3), while upon approaching jamming these same modes become increasingly delocalized.

FIG. 4.   IPR for $N = 8192$ particles in $d = 4$–7, averaged over 30 to 50 configurations, (a) moderately compressed $\Delta\phi/\phi_J \approx 0.2$ and (b) highly compressed $\Delta\phi/\phi_J \approx 1.4$ above jamming. Statistical errors are comparable to the data scatter.

Delocalization in this limit, however, is never complete. In order to observe further IPR decrease, one must consider higher-dimensional systems (Fig. 4). Going from $d = 4$ to 7, as expected for the reason mentioned above, systematically decreases the degree of localization for all $\Delta\phi$. Upon reaching $d = \infty$ the spheres are expected to behave equivalently to the perceptron. Localized modes are thus related to low-dimensional structure; their precise geometrical origin, however, remains the object of active study [30,32].

Conclusion.—Our analysis reconciles the DOS of amorphous solids from the perceptron and effective medium theory [20,21], on the one hand, and simulation results in $d = 2$ and 3 [23,24], on the other. The key observations are twofold: (i) mean-field scaling of the DOS is robustly observed in all dimensions for $\Delta\phi/\phi_J \lesssim 1$, (ii) delocalization of low-frequency modes increases as $\Delta\phi/\phi_J \rightarrow 0$ and as $d \rightarrow \infty$. A boson peak contribution whose origin is purely mean field in nature therefore exists in amorphous solids even far from jamming, while quasilocalized modes are a low-dimensional effect whose origin is likely related to specific geometrical features [32]. Because some of the structural features of configurations at ϕ_J, notably rattlers and bucklers, vanish exponentially as d increases [27,28], we tentatively conclude that quasilocalized modes also cannot be obtained perturbatively from mean-field, infinite-dimensional descriptions. We also conclude that the existence of a boson peak is independent of quasilocalization proper, in contrast to Ref. [11].

Another interesting feature of the DOS is observed for $\Delta\phi/\phi_J \gtrsim 1$. Even though the results remain largely independent of dimension, they are quite distinct from the mean-field scaling form that easily describes the $\Delta\phi/\phi_J < 1$ regime. Whether this effect is due to a breakdown of some of the assumptions made in the comparison or to the presence of a phase transition at $T = 0$ as has recently been proposed [33] remains, however, an open question.

Data relevant to this work have been archived and can be accessed at [34].

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