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Long-wavelength structural anomalies in jammed systems

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The structural properties of static, jammed packings of monodisperse spheres in the vicinity of the jamming transition are investigated using large-scale computer simulations. At small wave number k, we argue that the anomalous behavior in the static structure factor, $S(k) \sim k$, is consequential of an excess of low-frequency, collective excitations seen in the vibrational spectrum. This anomalous feature becomes more pronounced closest to the jamming transition, such that $S(0) \to 0$ at the transition point. We introduce an appropriate dispersion relation that accounts for these phenomena that leads us to relate these structural features to characteristic length scales associated with the low-frequency vibrational modes of these systems. When the particles are frictional, this anomalous behavior is suppressed providing yet more evidence that the jamming transitions for frictional spheres lie at lower packing fractions than for frictionless spheres. These results suggest that the mechanical properties of jammed and glassy media may therefore be inferred from measurements of both the static and dynamical structure factors.

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I. INTRODUCTION

The emergence of similarities between the properties of molecular glasses, dense colloidal suspensions, foams, and granular materials has led to the notion of jamming [1]—the transition between solidlike and fluidlike phases in disordered systems—as a manner through which one can gain a deeper understanding of the traditional liquid-glass transition and the fascinating, complex phenomena observed in amorphous materials in general [2]. Although there have recently been some works highlighting the differences between the onset of rigidity in jammed matter and glassiness [3,4], the emphasis in this work is on the commonalities between the two [5–8]. Here, we aim to provide a heuristic physical picture that accounts for specific, long-wavelength, structural features that emerge in the jammed state and relate these features to their dynamical properties.

Donev *et al.* [9] found that in the *hard-sphere* jamming transition, the structure factor, $S(k)$, exhibits a linear dependence on wave number $k \equiv |\mathbf{k}|$,

$$S(k) \propto k \quad \text{as} \quad k \to 0. \tag{1}$$

This behavior of $S(k)$ suggests that the total correlation function $h(r)$ decays as $|r^{-4}|$ at large separations r, as deduced from the asymptotic estimates of Fourier transforms [10–12]. Similarly, it suggests a long-range behavior for the direct correlation function $c(r)$. This is indeed in contrast to standard liquid state theory for liquids whose constituents interact via a finite range potential—hence $c(r)$ is short ranged—which predicts $S(k) \propto k^2$. This anomalous low-k behavior can be interpreted as being indicative of the suppression of long-wavelength density fluctuations due to hyperuniformity [13]. Here, we propose an alternative interpretation related to large length-scale collective dynamics.

This paper is arranged as follows. We provide a brief overview of the molecular-dynamics (MD) simulations used here to generate liquid and jammed states. We then review previous results from studies of the jamming transition pertinent to the discussion here. This is followed by a discussion on the relevant concepts from liquid state theories that indicate that our results and those of Ref. [9] for frictionless particles are indeed rather unusual. We then present our results for the static structure factor, $S(k)$, at small values of the wave number k, in our jammed, model glassy system. We then put forward a conjecture that relates the asymptotic behavior of $S(k)$ to an excess of vibrational modes relative to the Debye model. We end with results from ongoing work on frictional systems and conclusions.

II. SIMULATION MODEL

The computer simulations performed here are for monodisperse, *soft spheres* of diameter d and mass m, interacting through a finite range, purely repulsive, one-sided, harmonic potential

$$V(r) = \left\{ \begin{array}{ll} \dfrac{\varepsilon}{2d^2}(d-r)^2 & r < d, \\ 0 & r > d \end{array} \right\}, \tag{2}$$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ is the center-to-center separation between particles i and j located at $\mathbf{r}_i$. The strength of the interaction is parameterized by ε, which is set to unity in this study. Most of the results presented below are for frictionless particles, with friction coefficient $\mu = 0$. We also present preliminary results for frictional packings using a static friction model [14] to compare between frictionless and frictional systems. In the frictional packings, the particle friction coefficient was varied, $0.01 \leq \mu \leq 1.0$. We simulated systems ranging in size, $1024 \leq N \leq 256\,000$ particles, in cubic simulation cells of size $10d \lesssim L \lesssim 50d$, with periodic boundary conditions, over a range of packing fractions, $\phi = N\pi d^3/L^3$.

The jamming protocol implemented here to generate zero-temperature jammed packings is similar to other soft-sphere protocols [15,16]. Initially, starting from a collection of spheres randomly placed in the simulation cell at low packing fraction $\phi_i=0.30$, we compressed the system to a specified overcompressed state, $\phi=0.74$, minimizing the energy of the system in a steepest-descent manner. At this value of $\phi=0.74$, all the particles experience overlaps with several other particles—their contact neighbors. The packings are mechanically stable and disordered with no signs of long-range order. To generate packings at $\phi<0.74$, we then incrementally reduced ϕ in steps of $10^{-6}\leq\delta\phi\leq10^{-2}$, minimizing the energy after each step. This allowed us to accurately determine the location of the jamming transition where the system unjams at a packing fraction ϕ_c (see below), for *each independent realization*, down to an accuracy of 10^{-6} in ϕ for $N\leq 10\,000$ and an accuracy of 10^{-3} for $N>10\,000$. For the largest system, $N=256\,000$, we generated four independent configurations at each value of ϕ.

We also studied equilibrated liquids of frictionless spheres at a dimensionless temperature $T=0.01$. This value of T was chosen to compare and contrast our results between liquid and jammed states.

Our main tool of analysis is the static structure factor $S(k)$, which we obtain in the standard way as a direct Fourier transform of the particle positions

$$S(k)=\frac{1}{N}\left|\sum_{i=1}^{N}\exp(\imath\mathbf{k}\cdot\mathbf{r}_i)\right|^2. \tag{3}$$

Here, $\mathbf{k}$ is the reciprocal-lattice vector for the periodic simulation cell, which is restricted to $k\geq 2\pi/L$. Although the data is noisy at the lowest wave numbers, our largest packings ($N=256\,000$) display the anomalous low-k behavior, as described below, well above the noise level. Throughout this study, $d=m=\varepsilon=1$ and all quantities have been appropriately nondimensionalized.

III. REVIEW

A. Jamming transition

Frictionless, purely repulsive, soft-sphere systems have been shown to undergo a zero-temperature transition between jammed and unjammed phases as a function of density or packing fraction [6,15–19]. In the infinite-size limit, this transition occurs at a packing fraction coincident with the value often quoted for random close packing, $\phi_{rcp}=0.64$ [6]. Above the jamming threshold $\phi>\phi_c$, the jammed state is mechanically stable to perturbations with nonzero bulk and shear moduli, whereas below the transition $\phi<\phi_c$, it costs no energy to disturb the system [18]. The relevant parameter here is not the absolute value of the packing fraction, rather the *distance* to the jamming transition defined through, $\Delta\phi\equiv\phi-\phi_c$. Thus, as a jammed state is brought closer to the transition point, $\Delta\phi\rightarrow0$, it gradually loses its mechanical rigidity and becomes increasingly soft. Intriguingly, this loss of mechanical stability as the jamming transition is approached can be related to diverging length scales [7] that characterize the extent of soft regions that determine the macroscopic behavior of system [20]. Experiments [21] have also identified growing length scales in the vicinity of the jamming transition thus promoting the idea that the jamming transition can be considered in the context of critical phenomena.

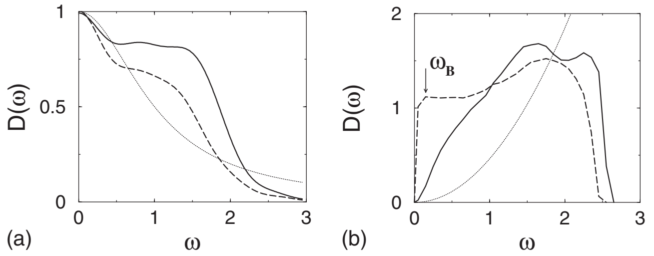

FIG. 1. The vibrational density of states, $\mathcal{D}(\omega)$, for two systems of $N=1024$ soft, frictionless spheres, characterized by the distance $\Delta\phi\equiv\phi-\phi_c$, from their zero-temperature, jamming transition packing fraction. Solid line: $\Delta\phi=1\times10^{-1}$. Dashed line: $\Delta\phi=1\times10^{-4}$. (a) Equilibrated liquids at $T=0.01$, well above their respective freezing or apparent glass transition temperatures. Data obtained from Fourier transforms of velocity autocorrelation functions and have been rescaled such that the $\omega=0$ intercepts coincide. A Lorentzian function (dotted) corresponding to Langevin diffusion [23] is also shown. (b) Jammed packings at zero temperature. The location of the *boson peak* is identified as ω_B for $\Delta\phi=1\times10^{-4}$. In (b), the Debye result (dotted), corresponding to the system $\Delta\phi=0.1$, was generated using values for the bulk and shear moduli [6] and is shown for comparison.

In this paper, we connect the long-wavelength structural features observed in $S(k)$ to correlation lengths characterizing the typical length scale of collective, low-frequency vibrational modes in jammed, zero-temperature, disordered packings [7]. In Ref. [7], it was shown that the approach of the jamming transition in a soft-sphere packing is accompanied by a dramatic increase in the number of low-frequency vibrational modes over the expected Debye behavior. In traditional glasses, these excess low-frequency modes in the vibrational density of states, $\mathcal{D}(\omega)$, are often referred to as the *boson peak* [22] in reference to the peak observed when plotting $\mathcal{D}(\omega)/\omega^2$. For convenience, we also employ this language here. A detailed study of $D(\omega)$ for jammed sphere packings and the appearance of the so-called boson peak can be found in [7].

In Fig. 1, we compare the vibrational density of states for dense, soft-sphere liquids [Fig. 1(a)] and amorphous jammed solids, identifying the location of the boson peak, ω_B, for our jammed system [Fig. 1(b)]. The location of the boson peak tends to zero at the jamming transition point, i.e., $\omega_B\rightarrow0$, as $\Delta\phi\rightarrow0$ [7]. The two values of $\Delta\phi=1\times10^{-4}$ and 1×10^{-1} correspond to actual packing fraction values of $\phi=0.6405$ and 0.74, respectively, for sample configurations used to generate this data.

Associated with this excess in the vibrational density of states are two diverging length scales: the longitudinal correlation length, ξ_L, characterizing the scale of collective excitations of longitudinal modes contributing to the boson peak, while ξ_T characterizes transverse excitations. These correlation lengths scale with the boson peak position as [7,20]

$$\omega_B\propto\xi_L^{-1}\quad(L\text{:longitudinal modes}), \tag{4}$$

$$\omega_B \propto \xi_T^{-2} \quad (T\text{:transverse modes}). \tag{5}$$

Thus, when the Debye contribution, ω_D, is included, the corresponding dispersion relations become

$$\omega_L(k) - \omega_{D,L} \cong \beta k, \tag{6}$$

$$\omega_T(k) - \omega_{D,T} \cong \alpha k^2. \tag{7}$$

The preceding relations are only approximate, valid for low frequencies. They both contribute to the boson peak: the longitudinal term by modifying the slope in the Debye relation, whereas the transverse contribution contains an anharmonic term. We discuss the relevance of these results further below.

B. Analyticity of *S*(*k*)

In order to avoid any misunderstanding, we define the concepts of regular and singular in the following sense [10]. Assuming k to be a complex variable, for any three-dimensional system interacting with tempered pairwise, additive potentials, namely, when

$$\phi(r) : \frac{1}{r^{3+\eta}} \quad \text{as} \quad r \to \infty; \quad \eta > 0 \tag{8}$$

and therefore integrable, $|\int d\mathbf{r}\,\phi(r)| < \infty$. Then, the structure factor, in the long-wavelength limit, reads [12]

$$S(k) : A\rho|k|^{\eta} + F(k^2) \quad \text{as} \quad k \to 0, \tag{9}$$

where $\rho = \frac{N}{V}$ is the number density, A is a constant that depends on the thermodynamic properties of the equilibrium system, and F is an analytic function of k, regular in the neighborhood of $k=0$. Thus, the second term on the right-hand side of Eq. (9) is the regular contribution to $S(k)$, whereas the first term—originating from the potential of interaction—is the singular term.

For instance, when $\eta=3$, as in the attractive part of the Lennard-Jones potential,

$$S(k) = A\rho|k|^3 + F(k^2), \tag{10}$$

a result originally derived by Enderby *et al.* [24]. Thus, a linear behavior of the structure factor at small values of k corresponds to $\eta=1$. Physically, this would correspond to a charge-dipole interaction, which Chan *et al.* [25] have shown can only be present if *long-ranged* dipole-dipole interactions are also included. Thus, in the present work, the linear behavior of $S(k)$, at small k, does not come from the potential of interaction, as the finite-range harmonic potential used here will only give the regular contribution to $S(k)$. However, this does suggest that the anomalous low-k behavior originates in long-ranged correlations associated with the system.

IV. RESULTS

A. Frictionless spheres

We initially generated a number of overcompressed, $\phi > \phi_c$, zero-temperature packings at various distances, $\Delta\phi \equiv \phi - \phi_c$, from the jamming transition point. We also point out that the main distinction between this work and that of Ref. [9] is that we study soft spheres and approach the jamming transition from above, $\phi \to \phi_c^+$, whereas, hard spheres necessarily approach the transition from below. In Fig. 2, we show $S(k)$ for two soft-sphere systems at $T=0.01$, well above their respective apparent glass transition temperatures T_g. [The corresponding densities of states are shown in Fig. 1(a).] For $\Delta\phi=10^{-1}$, $T_g<0.001$, while for smaller $\Delta\phi$, T_g lies below this. Qualitatively, the curves are similar. We find the usual primary peak corresponding to nearest neighbors and, as expected from standard liquid state theory [12,23], at lower k, $S(k) \propto k^2$, with a nonzero intercept at $k=0$, which corresponds to the finite compressibility sum rule [Fig. 2 inset]. Thus, for equilibrated liquids, the structure factor and the long-wavelength limit are quite insensitive to the location of the zero-temperature jamming transition at these values of the number density, $\rho \equiv N/L^3 = 6\phi/\pi d^3 = 1.22, 1.44$ for $\phi=0.6405$ $(\Delta\phi = 1\times10^{-4})$, $0.74(\Delta\phi=1\times10^{-1})$, respectively.

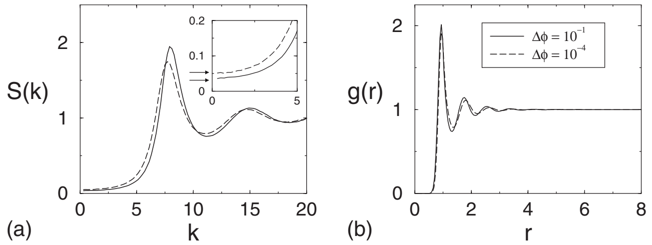

FIG. 2. Two $N=10\,000$ soft-sphere systems in the liquid state, $T=0.01$, for $\Delta\phi=1\times10^{-1}$ and 1×10^{-4} [see legend in panel (b)]. This temperature is well above the respective glass transition temperatures for the two systems, $T \gg T_g$. (a) Static structure factor $S(k)$, as a function of wave number k. The inset is a zoom of the region near the origin, where the arrows indicate the nonzero intercepts as $k\to0$. (b) Radial distribution function, $g(r)$, shows a prominent nearest-neighbor peak at $r\approx1$ and correlations that die off rapidly.

Turning our attention to the jammed phases at zero temperature [26], in Fig. 3, we show the radial distribution function $g(r)$ and the low-k region of $S(k)$, for $N=256\,000$ soft-spheres systems at three values of $\Delta\phi=1\times10^{-1}$, 1×10^{-2}, and 3×10^{-3}. Note that in Fig. 3(a), we use log-log scales to clearly demonstrate the linear region in $S(k)$. Far from the jamming transition, $\Delta\phi=1\times10^{-1}$, $S(k)$ plateaus near $k\approx1$ and tends to constant as $k\to0$. For the systems closer to the jamming transition, $\Delta\phi=1\times10^{-2}$ and $\Delta\phi=3\times10^{-3}$, there is a *qualitative change* in the low-k behavior of $S(k)$. We find a linear region, $S(k)\sim k$, extending over almost 1 order of magnitude at low k. We also point out that on closer inspection, the linear region extends to lower k for the system closest to the jamming transition point $(\Delta\phi=3\times10^{-3})$. At the smallest k attainable, $S(k)$ flattens out again because the system is not exactly at $\Delta\phi=0$. The radial distribution function shown in Fig. 3(b) exhibits typical features characteristic of a glassy phase; namely, a split second peak and additional shoulder on the third peak.

For completeness, we examine the influence of system size on the results presented here. In Fig. 4, we show $S(k)$ at $\Delta\phi\approx3\times10^{-3}$ for three different system sizes, $N = 1000, 10\,000, 256\,000$, corresponding to $L\approx10, 20, 60$. The main panel of Fig. 4 shows that the gross properties of

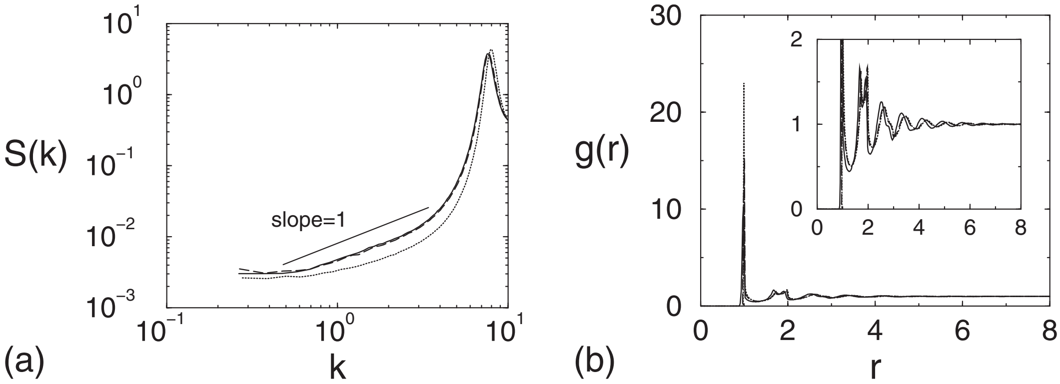

FIG. 3. Zero-temperature, jammed packings containing $N=256\,000$ purely repulsive, frictionless, soft-spheres at three different values of $\Delta\phi=1\times10^{-1}$ (dotted line), 1×10^{-2} (dashed), and 3×10^{-3} (solid). (a) Static structure factor $S(k)$. Far from the jamming transition, $\Delta\phi=1\times10^{-1}$, $S(k)$ plateaus nears $k\approx1$. Closer to jamming, $\Delta\phi=1\times10^{-2}$ and $\Delta\phi=3\times10^{-2}$, $S(k)$ exhibits approximately linear dependence on k over almost 1 order of magnitude in k, extending down to low k. A linear curve on this log-log plot is shown for comparison. (b) Radial distribution function. The jamming transition is characterized by a diverging nearest-neighbor peak at $r\approx1$, a clear splitting of the second peak [8], and oscillations that persist out to larger r than for the liquid state.

$S(k)$ do not depend on system size. Oscillations in $S(k)$ persist out to the largest k and is a consequence of the diverging nearest-neighbor peak in $g(r)$ [8]. The inset to Fig. 4 indicates that the linear portion of $S(k)$ at small k becomes resolvable for $N\geq10\,000$.

Thus, the first aim of this work shows that, similarly to the findings in Ref. [9], for hard spheres just below the jamming transition point, for our soft-sphere packings above ϕ_c, $S(k)$ exhibits a linear behavior at small values of momentum transfer. Hence, this unusual behavior not only pertains to hard spheres, but also to soft spheres, both above and below the jamming transition point, and possibly to finite-range repulsive potentials in general. We will attempt below to produce what we believe is a reasonable explanation for the origin of this behavior which, as stated at the beginning, does appeal to a conjecture.

Since, in the long-wavelength limit, the linear behavior of $S(k)$ cannot arise from the singular contribution of the potential used in this work [12,24], it can only be due to the collective excitations present in the jammed or glassy state [27]. The collective excitations we have in mind are the same that are responsible for the boson peak. The range of k, over which $S(k)\sim k$, characterizes the length scale over which these excitations may be considered collective. As one approaches the jamming transition, this length scale diverges, a result consistent with work on the density of states of jammed packings [7].

Recent work by Chumakov *et al.* [28] did indeed show that the excitations leading to the boson peak are predominantly collective, in agreement with inelastic neutron-scattering experiments [29]. Although there have been a number of theories put forward [30–32], there is, at present, no agreed explanation as to the origins of the boson peak. For the purposes of this work, this is not necessary, except insofar as there is agreement that these excitations are predominantly collective and that the vibrational modes are likely to be kinetically driven. The arguments that follow are somewhat oversimplified, but we believe they are along the correct lines.

The following comments are in order: (i) In a system that undergoes the liquid-glass transition, the long-wavelength limit of the static structure factor, $S(k\rightarrow0)$, is not the thermodynamic compressibility κ_T, but a different value, say κ, which can actually be extracted from experiments [33]. (ii) Independently of the model or approximation used, the density fluctuations in the glass phase are kinetically, not thermodynamically, driven [33]. (iii) In spite of their different origins, the kinetic temperature, say T_{dyn}, defined for glasses, matches the Edwards temperature, T_{Edw}, used in granular matter. They happen to coincide within mean-field theories when the glass is in contact with an almost zero-temperature heat bath and the athermal grains are jammed [34].

The connection between the dispersion relations and the structure factor follows from the second moment of the dynamical structure factor, $S(k,\omega)$ [35],

$$2\int_0^\infty d\omega\omega^2 S(k,\omega)=\nu_0^2k^2, \tag{11}$$

where $\nu_0=\nu_0(T)$ (for a system in thermodynamic equilibrium $\nu_0^2=\frac{k_BT}{m}$, where k_B is Boltzmann's constant). The static structure factor is the zero moment of $S(k,\omega)$,

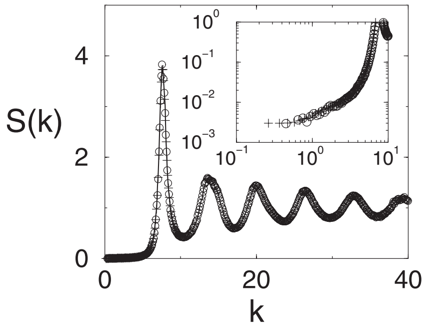

FIG. 4. $S(k)$ at $\Delta\phi\approx3\times10^{-3}$ for different systems sizes $N=1000$ (line), $N=10\,000$ (○), and $N=256\,000$ (+). Oscillations persist out to large k, reflecting the dominant nearest-neighbor peak in $g(r)$ shown in Fig. 3. Inset indicates that the linear behavior at low k becomes better resolved with increasing system size.

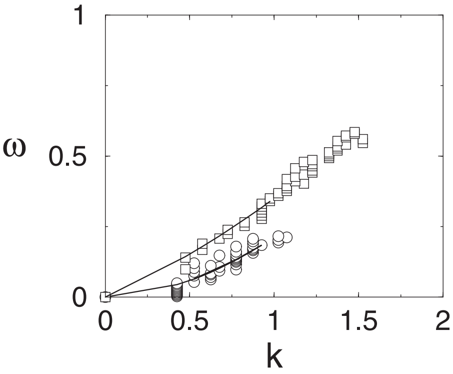

FIG. 5. Transverse dispersion behavior for $\Delta\phi = 10^{-1}$ (□) and 10^{-6} (○). Solid lines correspond to quadratic fits to the data as in Eq. (7). Data obtained from the low-frequency portion of the transverse structure factors of the vibrational modes for $N = 10\,000$.

$$S(k) = \int d\omega S(k,\omega). \tag{12}$$

We now put forward the following conjecture: assume that there is only one very well-defined collective mode with dispersion relation $\omega_B(k)$, the boson peak. This gives us a relation between the asymptotic long-wavelength behavior of $S(k)$ and the boson peak

$$S(k,\omega) = S(k)\,\delta[\omega - \omega_B(k)], \tag{13}$$

whence

$$S(k) = \nu_0^2 \frac{k^2}{2\omega_B^2(k)}. \tag{14}$$

This collective mode is associated with vibrational excitations with a wavelength of the order of the correlation length of the jammed state. We expand the dispersion relation at these small values of momentum transfer [27]

$$\omega_B(k) \cong ck + ak^2 + \cdots. \tag{15}$$

In Eq. (15), c is the speed of sound and the second term on the right-hand side denotes departures from the usual Debye behavior, such that both c and a are independent of k. Replacing Eq. (15) into Eq. (14), in the limit of $k \to 0$, we find

$$S(k) = \frac{\nu_0^2}{2c^2}\left(1 - 2\frac{a}{c}k\right) + \mathcal{O}(k^2). \tag{16}$$

Thus, on comparing Eqs. (15) and (16) to Eqs. (6) and (7), it transpires that it is the transverse modes that contribute to the linear behavior of $S(k)$. On the other hand, the longitudinal components, Eq. (6), only contribute a constant term to $S(k)$, modifying the slope of the Debye relation.

We illustrate the differences in the dispersion behavior at two extreme values of $\Delta\phi = 10^{-6}$ and 10^{-1} in Fig. 5. These results were obtained from diagonalization of the dynamical matrix for systems with $N = 10\,000$ and then locating the peaks in the transverse components of the Fourier transforms of the eigenmodes—transverse-mode structure factors [36,37]—and then averaging over a small range of frequencies. Data shown in Fig. 5 distinguish between the regular, linear dispersion relation that dominates the dispersion behavior far from the jamming transition at $\Delta\phi = 10^{-1}$, while the quadratic contribution to the dispersion behavior is significant closer to the jamming transition, $\Delta\phi = 10^{-6}$.

From the analysis, we obtain the transverse speed of sound, c_t, as a fitting parameter. At these two compressions, $c_t \approx 0.26(\Delta\phi = 10^{-1})$ and $c_t \approx 0.023(\Delta\phi = 10^{-6})$. The actual values calculated from the bulk and shear moduli data [6] give $c_t \approx 0.28(\Delta\phi = 10^{-1})$ and $c_t \approx 0.018(\Delta\phi = 10^{-6})$. Therefore, we find reasonable agreement within this approximation. If we use only a linear dispersion relation, we find that the values of c_t computed here and the actual values [6] vary by as much as 1 order of magnitude. This can be realized by the observation that a linear fit to data for $\Delta\phi = 10^{-6}$ does not pass through the origin as required in the hydrodynamic limit.

The linear feature of $S(k)$ in the small-k regime appears here as a consequence of assuming an "excess" relative to the Debye model for the dispersion relation and only one collective mode. Although the "excess" model used here appears as an approximation appropriate for the low-k regime, we have reconciled this with existing results on the emergence of characteristic length scales associated with these collective excitations. More generally, however, it does suggest that the boson peak and the linear behavior of $S(k)$, as $k \to 0$, are two sides of the same coin. Therefore, this anomalous suppression of long-wavelength density fluctuations emerges as a consequence of large length-scale correlated dynamics in the low-frequency modes of the jammed solid. Furthermore, although the boson peak has been traditionally associated with the glassy phase, recent low-frequency Raman spectroscopic studies of glassy, supercooled, and molten silica reveal that the boson peak persists into the liquid phase [38]. This also appears to be the case with other network systems (see references in Ref. [38]) which, in the molten state, show a distinctive prepeak at small k in $S(k)$. This prepeak is indicative of intermediate-range order in those melts, representing a characteristic length in those melts that measures the correlations between the centers of "clusters" present in the liquid state. This intermediate-range clustering may in fact promote longer wavelength correlated dynamics in the liquid state. It may therefore be interesting to investigate experimentally, and by means of MD simulations, whether the low-k behavior of $S(k)$ in those systems is also linear both in their glassy and liquid phases.

B. Frictional packings

Studies on jammed packings of *frictional* particles are less well developed. The picture that is emerging is that frictional packings undergo a similar zero-temperature jamming transition at packing fractions which now become friction dependent [39–42]. In the limit of high friction coefficient, the frictional jamming transition coincides with the value associated with random loose packing, $\phi_{rlp} \approx 0.55$ +[41–45]. Thus the relevant parameter that measures the distance to the jamming transition now becomes a friction-dependent quantity, $\Delta\phi(\mu)$ [42].

We test these concepts through $S(k)$ for packings over a

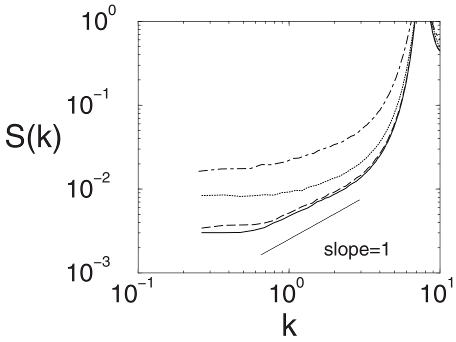

FIG. 6. Log-log plot of the static structure factor $S(k)$, focusing on the low-k region. All packings at the same $\phi=0.64$ contain $N=256\,000$ purely repulsive, monodisperse, soft spheres with different friction coefficients $\mu=0$ (solid line), 0.01 (dashed), 0.1 (dotted), and 1.0 (dot-dashed).

range of friction coefficients at the *same* $\phi=0.64$, which translates to different values of $\Delta\phi(\mu)$. Our preliminary results in Fig. 6 are data for $S(k)$ for jammed packings with $0\leq\mu\leq 1$. At this fixed value of $\phi=0.64$, $\Delta\phi(\mu)$ increases with increasing friction coefficient. Therefore, we expect that the anomalous linear behavior in the low-k region of $S(k)$ should become less prominent with increasing μ. Indeed, this trend is observed in Fig. 6, thus providing yet further evidence that the jamming transition point shifts to lower ϕ with increasing friction. To recover the linear behavior at low k in frictional packings, we would therefore need to study mechanically stable packings at lower ϕ. This work in ongoing.

V. CONCLUSIONS

In conclusion, we have provided a physical, albeit naive, explanation for the observation of the apparent suppression of long-wavelength density fluctuations in jammed model glassy materials. We submit that it is the presence of low-frequency, collective excitations, mainly of transverse character, contributing to the excess of low-frequency modes, that are responsible for the linear behavior at low k in $S(k)$. The relevant length scale here is the transversal correlation length that contributes to the diverging boson peak in the jammed phase. This low-k feature is most pronounced in the model system studied here for soft particles at packing fractions above the zero-temperature jamming transition matching the behavior on the other side of the jamming transition for hard spheres. This connection between the long-wavelength behaviors on either side of the transition reinforces the view that the jamming transition is critical in nature. Although we also point out that the jamming transition is very different from a thermodynamic liquid-gas critical point in that we do not observe a divergence in $S(k=0)$, but rather it becomes zero.

Moreover, we expect that as the transition is approached,

$$\nu_0(\mathcal{T}) \to 0 \Rightarrow S(0) \to 0 \quad \text{as } \Delta\phi \to 0. \qquad (17)$$

The dependence of $\nu_0(\mathcal{T})$ on a generalized temperaturelike quantity, $\mathcal{T}$, in jammed packings is consistent with the concept of the *angoricity* [46,47]. This plays the role of temperature in packings of elastic particles and goes to zero when the particles fall out of contact which occurs at the jamming transition. Future studies may also provide a way to understand the connection between different temperature definitions relevant to the study of thermal and jammed systems. Our preliminary data for frictional packings also provide further evidence that the location of the jamming transition occurs at lower packing fractions with increasing friction coefficient. The underlying nature of the low-frequency modes in frictional materials has yet to be investigated in three-dimensional systems and forms part of ongoing work. When friction is present, the modes will contain not only the translational character as seen in frictionless systems, but also rotational character due to the additional degrees of freedom.

This anomalous low-k behavior is also likely to be present in other, finite-range, model repulsive systems. These features may be detected, using the appropriate spectroscopy, in (hard-sphere) colloidal glasses and granular packings, which can be prepared close to their respective jamming transitions.

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[1] A. J. Liu and S. R. Nagel, Nature (London) **396**, 21 (1998).
[2] *Unifying Concepts in Granular Media and Glasses*, edited by A. Coniglio, A. Fierro, H. J. Herrmann, and M. Nicodemi (Elsevier, Amsterdam, 2004).
[3] R. Mari, F. Krzakala, and J. Kurchan, Phys. Rev. Lett. **103**, 025701 (2009).
[4] I. Biazzo, F. Caltagirone, G. Parisi, and F. Zamponi, Phys. Rev. Lett. **102**, 195701 (2009).
[5] C. S. O'Hern, S. A. Langer, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. **86**, 111 (2001).
[6] C. S. O'Hern, L. E. Silbert, A. J. Liu, and S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).
[7] L. E. Silbert, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. **95**, 098301 (2005).
[8] L. E. Silbert, A. J. Liu, and S. R. Nagel, Phys. Rev. E **73**, 041304 (2006).
[9] A. Donev, F. H. Stillinger, and S. Torquato, Phys. Rev. Lett. **95**, 090604 (2005).
[10] M. J. Lighthill, *Introduction to Fourier Analysis and Generalised Functions* (Cambridge Univeristy Press, Cambridge, England, 1978).
[11] G. Stell, in *Statistical Mechanics, Part A: Equilibrium Tech-*

niques, edited by B. J. Berne (Plenum Press, New York, 1977).
[12] J. H. Nixon and M. Silbert, J. Phys. C **15**, L165 (1982).
[13] S. Torquato and F. H. Stillinger, Phys. Rev. E **68**, 041113 (2003).
[14] L. E. Silbert, D. Ertaş, G. S. Grest, T. C. Halsey, D. Levine, and S. J. Plimpton, Phys. Rev. E **64**, 051302 (2001).
[15] H. A. Makse, D. L. Johnson, and L. M. Schwartz, Phys. Rev. Lett. **84**, 4160 (2000).
[16] H. P. Zhang and H. A. Makse, Phys. Rev. E **72**, 011301 (2005).
[17] D. J. Durian, Phys. Rev. Lett. **75**, 4780 (1995).
[18] C. S. O'Hern, S. A. Langer, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. **88**, 075507 (2002).
[19] W. G. Ellenbroek, E. Somfai, M. van Hecke, and W. van Saarloos, Phys. Rev. Lett. **97**, 258001 (2006).
[20] M. Wyart, L. E. Silbert, S. R. Nagel, and T. A. Witten, Phys. Rev. E **72**, 051306 (2005).
[21] F. Lechenault, O. Dauchot, G. Biroli, and J.-P. Bouchaud, Europhys. Lett. **83**, 46003 (2008).
[22] *Amorphous Solids, Low Temperature Properties*, edited by W. A. Phillips (Springer, Berlin, 1981).
[23] D. A. McQuarrie, *Statistical Mechanics* (University Science Books, Sausalito, 2000).
[24] J. E. Enderby, T. Gaskell, and N. H. March, Proc. Phys. Soc. London **85**, 217 (1965).
[25] D. Y. C. Chan, D. J. Mitchell, B. W. Ninham, and B. A. Pailthorpe, J. Chem. Phys. **69**, 691 (1978).
[26] Because we use monodisperse spheres, we do not attempt to gradually cool the system towards the glass temperature, rather we analyzed the jammed packings that were initially generated at specified values of $\Delta\phi$.
[27] C. C. Matthai and N. H. March, Phys. Chem. Liq. **11**, 207 (1982).
[28] A. I. Chumakov, I. Sergueev, U. van Burck, W. Schirmacher, T. Asthalter, R. Ruffer, O. Leupold, and W. Petry, Phys. Rev. Lett. **92**, 245508 (2004).
[29] C. Masciovecchio, A. Mermet, G. Ruocco, and F. Sette, Phys. Rev. Lett. **85**, 1266 (2000).
[30] S. N. Taraskin, Y. L. Loh, G. Natarajan, and S. R. Elliott, Phys. Rev. Lett. **86**, 1255 (2001).
[31] T. S. Grigera, V. Martin-Mayor, G. Parisi, and P. Verrocchio, J. Phys.: Condens. Matter **14**, 2167 (2002).
[32] M. Wyart, S. R. Nagel, and T. A. Witten, Europhys. Lett. **72**, 486 (2005).
[33] W. Gotze and L. Sjogren, Rep. Prog. Phys. **55**, 241 (1992).
[34] A. Barrat, J. Kurchan, V. Loreto, and M. Sellitto, Phys. Rev. E **63**, 051301 (2001).
[35] P. A. Egelstaff, *An Introduction to the Liquid State* (Academic Press, London, 1967).
[36] G. S. Grest, S. R. Nagel, and A. Rahman, Phys. Rev. Lett. **49**, 1271 (1982).
[37] L. E. Silbert, A. J. Liu, and S. R. Nagel, Phys. Rev. E **79**, 021308 (2009).
[38] A. G. Kalampounias, S. N. Yannopulos, and J. Papatheodorou, J. Non-Cryst. Solids **352**, 4619 (2006).
[39] K. Shundyak, M. van Hecke, and W. van Saarloos, Phys. Rev. E **75**, 010301(R) (2007).
[40] E. Somfai, M. van Hecke, W. G. Ellenbroek, K. Shundyak, and W. van Saarloos, Phys. Rev. E **75**, 020301(R) (2007).
[41] C. Song, P. Wang, and H. A. Makse, Nature (London) **453**, 629 (2008).
[42] L. E. Silbert (unpublished).
[43] G. Y. Onoda and E. G. Liniger, Phys. Rev. Lett. **64**, 2727 (1990).
[44] M. Jerkins, M. Schröter, H. L. Swinney, T. J. Senden, M. Saadatfar, and T. Aste, Phys. Rev. Lett. **101**, 018301 (2008).
[45] L. E. Silbert, D. Ertaş, G. S. Grest, T. C. Halsey, and D. Levine, Phys. Rev. E **65**, 031304 (2002).
[46] R. Blumenfeld and S. F. Edwards, J. Phys. Chem. B **113**, 3981 (2009).
[47] S. Henkes and B. Chakraborty, Phys. Rev. E **79**, 061301 (2009).