Spatial Distributions of Local Elastic Moduli Near the Jamming Transition

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Recent progress in studies of the nanoscale mechanical responses in amorphous solids has highlighted a strong degree of heterogeneity in the elastic moduli of thermal glassy systems. In this contribution, using computer simulations, we study the elastic heterogeneities in athermal amorphous solids, composed of isotropic, static, sphere packings near the jamming transition. We employ techniques based on linear response theory which avoid the need to invoke any explicit deformation. Not only do we validate these procedures by reproducing established scaling laws for the global elastic moduli, but our technique reveals new power-law behaviors in the spatial fluctuations of the local moduli. The local moduli are randomly distributed in space, and are described by Gaussian probability distributions all the way down to the transition point. However, the moduli fluctuations grow as the jamming threshold is approached, through which we are able to identify a characteristic length scale, associated with the shear modulus heterogeneities.

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I. INTRODUCTION

When traditional, crystalline solids are linearly deformed, their responses are typically described by affine deformations. This type of reasoning leads to classical theories such as those of isotropic, linear elasticity [1]. Contrary to this, disordered solids, such as thermal amorphous solids, i.e. glasses, disordered crystals [2], as well as athermal jammed solids [3], exhibit strongly non-affine responses. This non-affine characteristic becomes significantly apparent during shear deformation [4]. Under shear, the constituent particles undergo additional non-affine displacements [5], leading to a decrease in the shear modulus. The differences observed between the zero-time, i.e. only affine, and the infinite-time shear moduli suggest that it is this non-affine character that dominates the shear modulus on approach to the jamming transition, where a mechanically stable solid loses its rigidity [6].

The appearance of non-affine response is closely related to elastic heterogeneities [7], especially spatially varying shear moduli. Indeed, DiDonna and Lubensky [8] proposed that non-affine displacements of particles subject to shear are driven by randomly fluctuating local elastic moduli. Amorphous solids reflect just such inhomogeneous behavior in their mechanical responses at the nanoscale, as seen in both computer simulations [9] and experiments [10]. Manning and co-workers [10, 11] identified soft spots as regions of atypically large displacements in low-frequency, quasi-localized vibrational modes. Particle rearrangements, activated by mechanical load [11, 13] as well as by thermal energy [12, 14], are therefore understood to be spatially correlated with those soft spots, which can be linked to locally un-stable regions with negative shear moduli [9]. Ellenbroek et al. [15] showed that the non-affine responses in marginally jammed solids are caused by proximity to so-called floppy modes. As Wyart et al. [16, 17] suggested, these floppy modes are generated by weakly connected clusters of particles, which define regions of marginal stability within the bulk solid, and which can be also related to low moduli regions.

The focus of this study is the heterogeneities of local elastic moduli, paying particular attention to the local shear modulus, in model granular solids of isotropically compressed, static sphere packings. For these athermal systems, the temperature is effectively zero, \( T = 0 \), and the packing fraction \( \phi \) of particles is a control parameter that we use to systematically probe static packings of varying rigidity. We characterize rigidity by the distance, \( \Delta \phi = \phi - \phi_c \), from the jamming transition point \( \phi_c \), or equivalently the packing pressure, \( p \). The approach of \( \phi_c \) from above \( ( p \to 0^+ ) \) is governed by various power-law scalings with \( \Delta \phi \), as observed in simulations [3, 8, 15] and experiments [18], in quantities including the global elastic moduli. The novelty of the approach described here is that we measure the elastic moduli without resorting to explicit deformations, rather employing techniques derived from linear response theory [19, 21], and which proves to be a useful method to probe fragile systems.

II. NUMERICAL METHOD

Our numerical system is composed of mono-disperse, frictionless, inelastic spheres with diameter \( \sigma \) and mass \( m \), in 3 dimensions [21]. Particles interact via a finite-range, purely repulsive potential: \( V(r) = (\epsilon/a)(1-r/\sigma)^a \) for \( r < \sigma \), otherwise \( V(r) = 0 \), where \( r \) is the center-to-center separation between two particles. Here we show results for Hertzian contacts, \( a = 2.5 \), only [22]. Length, mass, and time are presented in units of \( \sigma \), \( m \), and

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\( \tau = (m \sigma^2 / \epsilon)^{1/2} \), respectively. We prepared 10 configurations of each of \( N = 1,000 \) and \( N = 10,000 \) particles, in periodic cubic simulation boxes over several orders of magnitude in packing pressure, \( 10^{-7} < p < 10^{-1} \), corresponding to \( 10^{-5} < \Delta \phi < 10^{0} \). For calculations of the local, and subsequently global, properties, we implemented the fluctuation formulae developed within linear response theory \([19, 20]\). Specifically, the harmonic approximation \( (T = 0) \) and the finite-temperature formulation \( (T = 10^{-9} \text{ to } 10^{-10}) \) were employed \([23]\); cf. Ref. \([24]\) for details of the formulation and implementation.

To probe local properties, the simulation box was divided into little domains of size \( w_x \times w_y \times w_z \), i.e. the coarse-graining (CG) domains. In each domain \( m \), we computed the local bulk modulus \( K^m \) and shear modulus \( G^m \) \([23]\). \( K^m, G^m \) consist of two components: those attributed to instantaneous affine deformations \( K_A^m, G_A^m \) and to non-affine deformations that contribute negatively to the overall modulus \( K^m, G^m \), \( K^m = K_A^m - K_N^m \) and \( G^m = G_A^m - G_N^m \) \([24, 28]\). We then calculated the probability distribution function \( P(X^m) \) for the moduli \( X^m = K^m, G^m \), from which the average, \( \bar{X} = \int \! X \, P(X^m) \, dX^m \), and the standard deviation (SD), \( \sigma_X = \int \! (X - \bar{X})^2 \, P(X^m) \, dX^m \), were obtained. \( \delta X = \delta X(p, w_x, w_y, w_z) \) depends on both \( p \) and the size of the CG domain, whereas \( X = X(p) \) corresponds to the global value, independent of \( w_x, w_y, w_z \).

**III. RESULT**

Figure 1 shows the dependence on pressure, \( p \), for the global \( X(p) \) in the top panels, (a) and (d). Our techniques, both the \( T = 0 \) and \( T > 0 \) protocols, reproduce values and scaling results consistent with previous studies on similar systems \([8, 14, 15]\). Thus, our procedures allow us to obtain global bulk, \( K \), and shear, \( G \), modulus information from static packings. We also find that the global pressure (not shown) scales as, \( p \sim \Delta \phi^{1.5} \), for \( a = 2.5 \) (Hertzian contacts). Thereby, in the following, we present our scaling results in terms of \( \Delta \phi \) using this conversion factor. Thus, we find the scaling laws for \( X \) normalized by the effective spring constant \( k_{\text{eff}} \sim V'' \sim \Delta \phi^{a-2} \) \([29]\), \( X/k_{\text{eff}} \), are consistent with:

\[
K/k_{\text{eff}} \sim \Delta \phi^0, \quad G/k_{\text{eff}} \sim \Delta \phi^{0.5}.
\]  

(1)

The middle panels, Fig. 1(b), (e), show the absolute fluctuations, \( \delta X(p, w_x, w_y, w_z) \), where the CG domain is cubic of linear size, \( w_x = w \simeq 3 \) (\( \alpha = x, y, z \)), and from which we find,

\[
\delta K/k_{\text{eff}} \sim \Delta \phi^0, \quad \delta G/k_{\text{eff}} \sim \Delta \phi^{0.27}.
\]  

(2)

The bottom panels, (c) and (f), present the fluctuation data on a relative scale, \( \delta X/X \). As \( \Delta \phi \rightarrow 0 \) \( (p \rightarrow 0) \), \( \delta K/K \) approaches a constant value \([30]\), whereas relative fluctuations of the shear modulus grow as

\[
\delta G/G \sim \Delta \phi^{-\nu_G}, \quad \nu_G \simeq 0.5 - 0.27 = 0.23.
\]  

(3)

**FIG. 1.** (Color online) The average (global) value \( X \) and standard deviation \( \delta X \) of the probability distribution \( P(X^m) \) for \( X^m = K^m \) (bulk modulus) in (a)-(c) and \( G^m \) (shear modulus) in (d)-(f). The values of \( X, \delta X \), and their ratio \( \delta X/X \) are plotted as functions of pressure \( p \). The CG domain is cubic of linear size \( w_x = w \simeq 3 \) (\( \alpha = x, y, z \)). The open and closed symbols represent values from the harmonic approximation \( (T = 0) \) and the finite \( T > 0 \) formulation \( (T = 10^{-9} \text{ to } 10^{-10}) \), respectively, which coincide at \( p > 10^{-5} \) within numerical accuracy. The values for the affine and non-affine components are also plotted. Lines represent power-law scalings with \( p \), which are converted to those in \( \Delta \phi \) using \( p \sim \Delta \phi^{1.5} \) in the main text.

We now turn to a more explicit view of the spatial distributions of the local moduli \( K^m \) and \( G^m \). Figure 2 presents the probability distributions \( P(K^m) \) in (a) and \( P(G^m) \) in (b). These distributions are well-characterized as Gaussians over the range, \( 10^{-7} < p < 10^{-1} \) (see also (c) and (d)). However, here we point out that \( G^m \) contains negative values, whereas all the \( K^m \) are positive. The fraction of negative shear modulus regions, which is quantified by \( F_n = \int_{G^m < 0} P(G^m) \, dG^m \), increases as \( p \rightarrow 0 \), as shown in the inset of Fig. 2(b). \( F_n \approx 0.3 \) at the lowest \( p = 4 \times 10^{-7} \) indicates that 30% of the system is mechanically unstable, which are stabilized by remaining the 70% of stable regions \([9]\). This trend suggests that precisely at the transition \( \phi_c \) \( (p = 0) \), we expect to find a \( 1:1 \) ratio of stable and unstable regions that are just balanced, thus confirming the notion that the system is...
FIG. 2. (Color online) Probability distributions $P(X^m)$ and spatial correlation functions $C_{X^m}(r)$ of $X^m = K^m, G^m$ for the range of $p$. Distributions for, (a) $K^m$ and (b) $G^m$, and the relative fluctuations to the global values, (c) $K^m = (K^m - K)/K$ and (d) $G^m = (G^m - G)/G$. Spatial correlation functions (defined in main text) for, (e) $K^m$ and (f) $G^m$. The inset to (b) shows the fraction of negative $G_m$ regions, $F_0 = \int_{G_m < 0} P(G^m)dG^m$, as a function of $p$. In (a)-(d), solid lines indicate Gaussians. In (e),(f), vertical lines indicate the CG length, $r = w_x = w \simeq 3$.

Indeed fragile [31] with the global $G \to 0$.

In the middle panels (c),(d) of Fig. 2 we plot $P(K^m)$ and $P(G^m)$ of the relative fluctuations of the moduli, $X^m = (X^m - X)/X$. We recognize that $P(G^m)$ broadens as $p$ decreases, which is quantitatively demonstrated by $\delta G/G$ in Fig. 1(f) [32]. While variations in $P(K^m)$ are rather small and insensitive to $p$, as is consistent with $\delta K/K$ in Fig. 1(c) (note the scales are different between $K^m$ and $G^m$ in Figs. 2(c),(d)). In an effort to directly detect a correlation length associated with these fluctuations, the bottom panels (e),(f) of Fig. 2 show the spatial correlation functions of the fluctuations, $C_{X^m}(r) = \langle \hat{X}^m(r)\hat{X}^m(0) \rangle_0 / \langle \hat{X}^m(0)\hat{X}^m(0) \rangle_0$, where we explicitly represent $\hat{X}^m$ as a function of the position $r$, and $\langle \rangle_0$ denotes the spatial average over the position $0$. Both $C_{K^m}(r)$ and $C_{G^m}(r)$ decay with the CG length

$$r = w_x = w \simeq 3.$$  

This observation indicates that $K^m$ and $G^m$ fluctuate randomly in space without any apparent correlation, which, remarkably, persists down to the transition point. Indeed, thermal glasses [9, 24, 32] as well as disordered crystals [27, 28] similarly exhibit random spatial distributions in their local moduli that are similarly Gaussian.

An alternative view to determining a possible characteristic length scale is through the dependence of the fluctuations, $\delta G/G$, on the size of the CG domain, $w_x \times w_y \times w_z$. Here we consider three different ways to vary the CG domain: we vary (i) $w_x, w_y, w_z$ equally so that, $w_x = w_y = w_z = w$, (ii) $w_x, w_y$ as $w_x = w_y = w$, keeping fixed, $w_z \simeq 3$, (iii) only $w_x$ as $w_x = w$, keeping fixed $w_y = w_z \simeq 3$. In (i), the CG domain is always cubic, whereas it becomes rectangular parallelepiped in (ii) and (iii). We can define the dimension $d_w$ of the CG domain, i.e., (i) $d_w = 3$, (ii) $d_w = 2$, and (iii) $d_w = 1$. Figure 3 shows the CG length $w$-dependence of $\delta G/G$ at several different $p$, for $d_w = 3$ in (a) and $d_w = 2$ in (b). As $w$ increases, the $P(X^m)$ become narrower, characterized by smaller $\delta X$, as the local values tend towards their global, macroscopic values [9, 24, 32]. For all pressures, $\delta G/G \sim w^{-1.4}$ for $d_w = 3$, and $\sim w^{-0.93}$ for $d_w = 2$, in addition, $\sim w^{-0.47}$ for $d_w = 1$ (not shown), where the exponents of 1.4, 0.93, 0.47 are consistent with $d_w/2$, and similar values are also found in $\delta K/K$. A similar power-law dependence on $w$ has also been reported for glasses, with exponent 1 in $d_w = 2$ [32] and 1.5 in $d_w = 3$ [24]. Thus, the relative fluctuations satisfy the following scaling behavior,

$$\delta X/X \sim w^{-d_w/2},$$  

which can be understood within the framework of a sum of random variable $X^m$ with Gaussian $P(X^m)$ [33, 34].

Combining the scaling results for $\delta G/G$ (Eqs. 3 and 4)
suppressed. Close to the transition, appears quite uniform, and large-scale fluctuations are apparent in systems that are very different. Further from the transition, (d) case of Fig. 2(d). There are large soft regions, \( \hat{\xi} \) scale, modulus are suppressed over sufficiently large CG lengths, and (c) small \( p = 4 \times 10^{-5} \) and large \( w \approx 6.5 \). In the figures, we plot the fluctuation relative to the global value, \( \hat{G}^m = (G^m - G) / G \), as a function of the position \((x, y)\). Note that the probability distribution function \( P(\hat{G}^m) \) for \( w \approx 3 \) ((a),(b)) is presented in Fig. 2(d).

\[
\xi_G \sim \Delta \phi^{-\nu_G}, \quad \nu_G = \nu_G / (d_w / 2).
\]

Note that the exponent \( \nu_G \) depends on the dimension \( d_w \). The idea of the length \( \xi_G \) associated with growing \( \Delta G / G \) is best visualized in the spatial maps of Fig. 4 (for \( d_w = 3 \) case), which show the local fluctuations of the shear modulus as follows: Panels (a) and (b) of Fig. 4 compare the modulus maps of \( \hat{G}^m = (G^m - G) / G \) for a slice through the 3D packings at two different \( p \), for the same values of \( w = w_x = w_y = w_z \). In reference to Fig. 4(a) \((d_w = 3)\), these two points lie at different values of \( \Delta G / G \) along a vertical line at \( w \approx 3 \), that intersect the respective \( p \) curves. At this value of \( w \), the two systems appear very different. Further from the transition point, \( p = 4 \times 10^{-2} \) (panel Fig. 4(a)), the system appears quite uniform, and large-scale fluctuations are suppressed. Close to the transition, \( p = 4 \times 10^{-5} \) (panel Fig. 4(b)), there are large soft regions, \( \hat{G}^m < 0 \), balanced by similarly large rigid regions, \( \hat{G}^m > 0 \). For the system closer to \( \phi_c \) (small \( p \)), the fluctuations become suppressed at the larger \( w = 6.5 \) (see Fig. 4(c)), so that the map resembles more the compressed system at the smaller value of \( w \). This is equivalent to drawing a horizontal line across Fig. 4(a) at the same value of \( \Delta G / G \) connecting the two curves of different \( p \).

**IV. CONCLUSION**

In conclusion, the approach of the jamming transition, where a system approaches a state of marginal stability, local shear modulus fluctuations relative to the global value increase as \( \delta G / G \sim \Delta \phi^{-\nu_G} \) (Eq. (5)). These growing fluctuations, which occur only for the case of the shear modulus, lead to the identification of a length scale \( \xi_G \sim \Delta \phi^{-\nu_G} \) (Eq. (5)) that characterizes the spatial extent of shear modulus heterogeneities. The exponent \( \nu_G = \nu_G / (d_w / 2) \) depends on the dimension \( d_w \) of the CG domain; \( \nu_G \approx 1 / 6 \) in \( d_w = 3 \), \( \approx 1 / 4 \) in \( d_w = 2 \), and \( \approx 1 / 2 \) in \( d_w = 1 \). In contrast, the isostatic length \( \xi_1 \) or the rigidity length scale \( \xi_r \) grow with an exponent 1/2. In addition, length scales diverging with an exponent 1/4 have been found in transverse vibrations \( \omega^2 \), heat transport \( D \), spatially correlated dynamics \( \xi_r \), elastic-granular crossover \( \xi_c \), and stability to boundary perturbation \( \xi_s \). What is apparent is that the characteristic length scale \( \xi_G \) indicates that a marginally stable solid can exhibit varying degrees of rigidity depending on the scale and the dimension of the domain over which it is probed.

As a final remark, our techniques to measure elastic moduli are amenable to the covariance matrix analysis and experimental procedure used to probe vibrational properties in dense packings \( \text{[11]–[14]} \). It might be worthwhile to check whether the shadow system, i.e., the Hamiltonian of an analog system of harmonic springs with stiffernes obtained from the covariance matrix, produces values of elastic moduli consistent with the original, exact system.

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[35] We determine the length scale $\xi_G$ as

$$\delta G/G = \alpha_0 (w/\xi_G)^{-d_w/2},$$

Eqs. [3] and [6] give Eq. [8], where the value $\xi_G$ itself depends on $\alpha_0$, but the exponent $\nu_G = \nu_G/(d_w/2)$ does not. We also define a length $\xi_K$ associated with $\delta K/K$, which converges to a constant value as $\Delta \phi \to 0$.

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