Non-Affine Displacements Below Jamming under Athermal Quasi-Static Compression

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Critical properties of frictionless spherical particles below jamming are studied using extensive numerical simulations, paying particular attention to the non-affine part of the displacements during the athermal quasi-static compression. It is shown that the squared norm of the non-affine displacement exhibits the power-law divergence toward the jamming transition point, and that the participation ratio of the displacements decreases near the transition point, meaning that the non-affine displacements become more localized. This can be interpreted from the development of the power-law tail of the distribution of the non-affine displacements. The critical exponents evaluated in two and three dimensions are different from each other, suggesting that the upper critical dimension below jamming is $d_{uc} > 2$, in contrast with above jamming where $d_{uc} \leq 2$.

Introduction.— When the density of constitute particles in a box is increased, the particles start to contact at a certain density, and a system suddenly acquires finite energy, mechanical pressure, and rigidity, without apparent structural changes $^1$. This phenomenon called jamming has been actively studied in recent years, and the onset is defined as the jamming transition point $\varphi_J$. The jamming transition is ubiquitously observed for very diverse athermal systems such as metallic bolls $^2$, forms $^3-^4$, colloids $^5$, polymers $^6$, candies $^7$, dices $^8$, biological tissues $^9$, growing microbes $^{10}$, and some neural networks $^{11-12}$.

A famous and popular numerical protocol to generate a jamming configuration is the athermal quasi-static compression (AQC), which combines the affine transformation with successive energy minimization $^{13}$. An advantage of this protocol is that one can unambiguously define the jamming transition point $\varphi_J$ as the packing fraction $\varphi$ at which the energy after the minimization has a finite value. With the AQC, extensive work has been done for frictionless, spherical, and purely repulsive particles above jamming $\varphi > \varphi_J$. The numerical studies uncovered that the critical exponents do not depend on the spatial dimensions $d$ for $d \geq 2$ $^{13-14}$, while different values of the critical exponents are reported for a quasi-one-dimensional system $^{15}$. The resultant critical exponents in $d \geq 2$ well agree with the mean-field predictions $^{16-18}$, suggesting that the upper critical dimension of the jamming transition is $1 < d_{uc} \leq 2$.

Somewhat surprisingly, the critical properties of the jamming transition below $\varphi_J$ during the AQC have not yet been fully investigated. One of the reasons is that the quantities showing the criticality above $\varphi_J$, such as the mechanical pressure, energy, and bulk/shear modulus, are trivially zero below $\varphi_J$, and other appropriate quantities are not necessarily clear below $\varphi_J$ $^{13}$. The criticality below $\varphi_J$ has been mainly investigated by adding thermal fluctuation $^{17-19}$, introducing a moving tracer $^{20}$, considering self-propelled particles $^{21}$, or quenching from random initial configurations $^{22-23}$. In particular, extensive work has been conducted on shear-driven systems $^{24-29}$. However, it would be more desirable if one can directly extract the criticality from the configurations during the AQC, without adding thermal fluctuations and external forces. A promising study in this direction has been done by Shen et al. $^{31}$, where it was showed that several physical quantities, such as the displacements of the particle positions, exhibit the rapid increase just below $\varphi_J$. However, the critical exponent below $\varphi_J$ and its dimensional dependence under the AQC have not been clarified yet.

In this work, we characterize the criticality below $\varphi_J$ during the AQC by investigating the statistical properties of the non-affine displacements. We first report the results in $d = 3$, where the mean-squared of the non-affine displacements diverges toward $\varphi_J$ with the critical exponent very close to that of the shear viscosity. By observing the participation ratio, it is shown that the displacements become more localized as the system approaches $\varphi_J$. The localization is a consequence of the development of the power-law tail of the distribution of the displacements. We also report the numerical results in $d = 2$ to discuss the dimensional dependence of the critical exponent. Our results show that the critical exponent in $d = 2$ differs from that in $d = 3$, suggesting that the upper critical dimension below $\varphi_J$ is $d_{uc} > 2$, in contrast with that of above $\varphi_J$ where $d_{uc} \leq 2$ $^{13-15}$.

Model.— The model mainly used in this work is frictionless spherical particles in $d = 3$. The interaction potential between $N$ particles is given as

$$V = \sum_{i<j}^{1,N} \frac{h_{ij}^2}{2} \theta(-h_{ij}, h_{ij} = |r_i - r_j| - R_i - R_j),$$

where $r_i = \{x_i, y_i, z_i\}$ and $R_i$ respectively denote the position and radius of the $i$-th particle. The particles are confined in a cubic box $r_i \in [0, L]^3$ with the periodic boundary conditions in all directions. To avoid crystallization, we use a binary mixture consisting of $N_S = N/2$ small particles and $N_L = N/2$ large particles. The radi
of large and small particles are $R_S = 0.5$ and $R_L = 0.7$, respectively. With those notations, the volume fraction $\varphi$ is written as

$$\varphi = \frac{2\pi N (R_S^3 + R_L^3)}{3L^3}. \tag{2}$$

**Numerics.**— Here we describe the AQC originally proposed by O’Hern et al. [13]. Starting from a random initial configuration at a small packing fraction $\varphi = 0.1$, compression and energy minimization are performed successively in sequence. For each step of the compression, the packing fraction is slightly increased as $\varphi \to \varphi + \varepsilon$ with $\varepsilon = 10^{-4}$, by performing the affine transformation $r_i \to r_iL(\varphi + \varepsilon)/L(\varphi)$, where $L(\varphi) = \left[2\pi N(R_S^3 + R_L^3)/3\varphi\right]^{1/3}$. Then, the energy is minimized by using the FIRE algorithm, for details see Ref. [32], until the energy or squared force becomes sufficiently small: $V_N/N < 10^{-16}$ or $\sum_{i=1}^N (\nabla_i V_N)^2/N < 10^{-25}$. The procedure is repeated up to the jamming transition point $\varphi_J$ at which $V_N/N > 10^{-16}$ after the minimization [13]. This algorithm determines the transition point $\varphi_J$ for each sample with an accuracy of $\varepsilon$. After obtained $\varphi_J$, we rerun the numerical simulation with the same initial configuration, which allows us to calculate the physical quantities as a function of $\delta \varphi \equiv \varphi_J - \varphi$. We only use the data for $\delta \varphi \gg \varepsilon$ so that the accuracy of $\varphi$ does not affect the results.

We perform the numerical simulations for various system sizes $N = 128, 256, 512, 1024, 2048$, and 4096. To improve the statistic, we average over 1000 samples for $N = 128$ and 256, and 100 samples for the other system sizes.

**Mean squared displacement.**— When the system is compressed from $\varphi$ to $\varphi + \varepsilon$, the displacement of the $i$-th particle can be written as

$$r_i(\varphi + \varepsilon) - r_i(\varphi) = \delta r_i^A + \delta r_i^{NA} \tag{3}$$

where $\delta r_i^A = [L(\varphi + \varepsilon)/L(\varphi) - 1] r_i(\varphi)$ and $\delta r_i^{NA}$ respectively denote the affine and non-affine parts of the displacement. In this work, we only focus on the non-trivial part of the displacement $\delta r_i^{NA}$.

To characterize the criticality of the non-affine displacements, we first observe the mean squared displacement

$$\langle \Delta \rangle = \frac{1}{N} \sum_{i=1}^N \Delta_i, \tag{4}$$

with

$$\Delta_i = \frac{(\delta r_i^{NA})^2}{3\delta l^2}, \tag{5}$$

where $\delta l = L(\varphi + \varepsilon)/L(\varphi) - 1$ accounts for the change of the linear distance $L$ of the system. In Fig. 1(a), we show $\langle \Delta \rangle$ as a function of $\delta \varphi = \varphi_J - \varphi$. For large $N$ and intermediate $\delta \varphi$, $\langle \Delta \rangle$ shows the power law

$$\langle \Delta \rangle \propto \delta \varphi^{-\beta}, \tag{6}$$

with

$$\beta = 2.5, \tag{7}$$

see the dashed line in Fig. 1(a). A recent numerical simulation reported the similar power law for the shear viscosity $\eta \sim \delta \varphi^{-2.55}$. [29]. We shall discuss a possible connection between $\langle \Delta \rangle$ and $\eta$ in the final section.

To further investigate the scaling of $\langle \Delta \rangle$, we perform a finite-size scaling analysis assuming the following scaling function:

$$\langle \Delta \rangle = N^\alpha D(N^{\alpha/\beta} \delta \varphi), \tag{8}$$

where $D(x) = O(1)$ for $x \ll 1$, and $D(x) \sim x^{-\beta}$ for $x \gg 1$. As shown in Fig. 1(b), a good scaling collapse is obtained with $\alpha = 1$. This result implies that the number of the correlated particles diverges as $N_{cor} \sim \delta \varphi^{-\beta}$, and the correlation length $L_{cor} \sim N_{cor}^{1/3} \sim \delta \varphi^{-\nu}$ with $\nu = \beta/3 = 0.83$ under the assumption that the correlated volume is compact. This is close to a previous result $\nu = 0.71$ obtained by the finite-size scaling analysis of the transition point [13].

**Participation ratio.**— To see the spatial structure of the displacements, we observe the normalized vector [33]:

$$e_i = \frac{\delta r_i^{NA}}{\sqrt{\sum_{i=1}^N (\delta r_i^{NA})^2}}, \tag{9}$$

which satisfies $\sum_{i=1}^N e_i \cdot e_i = 1$. In Fig. 2 we visualize $e_i$ by drawing spheres such that their radii are proportional to $|e_i|$. Far from jamming, the spatial distribution of $e_i$ is homogeneous and featureless, see Fig. 2(a). On the contrary, near jamming, a few particles have very large displacements, and thus the displacement is spatially heterogeneous and localized, see Fig. 2(d). We quantify the
\[ P = 0 \gamma P \]

- To investigate the degree of the localization by using the participation ratio:

\[ P = \frac{1}{N} \left( \sum_{i=1}^{N} e_i \cdot e_i \right)^2 \]

which (or inverse of which) is widely used in the study of condensed matter physics \[34\], including amorphous solids \[35, 36\]. If \( e_i \) is spatially localized to a single particle, say \( e_i \cdot e_i = \delta_{ii} \), the participation ratio \( P \) is proportional to \( N^{-1} \). On the contrary, if \( e_i \) is extended such that \( e_i \cdot e_i \sim N^{-1} \) for all \( i \), \( P \) is constant independent of \( N \). In Fig. 2 (a), we show the \( \delta \varphi \) dependence of \( P \). One can see that \( P \) decreases with approaching \( \varphi_f \) and increasing \( N \). To investigate the \( N \) dependence of \( P \), we use the following scaling form:

\[ P = N^{-\gamma} P(N^{1/3} \delta \varphi), \]

assuming the same correlated volume as in Eq. (8). We find a good collapse for \( \gamma = 0.27 \), see Fig. 2 (b). At \( \varphi_f \), \( P \) vanishes in the thermodynamic limit as \( P \sim N^{-\gamma} \) with \( \gamma = 0.27 \). This exponent relates to the fractal dimension \( d_f \) of \( e_i \), namely, if \( e_i \cdot e_i \sim L^{-d_f} \) for \( i = 1, \ldots, L^{d_f} \), this yields that \( P \sim N^{-1 + d_f/3} \) \[34\], leading to

\[ d_f = 3(1 - \gamma) = 2.19. \] (12)

Therefore, \( e_i \) has a more compact structure than the bulk \( d = 3 \). A mean-field theory of the jamming transition predicts that the correlated volume \( v_{col} \) and correlation length \( l_{cor} \) have the following relation \( v_{col} \sim l_{cor}^{2} \) \[37, 38\]. This may imply that the fractal dimension is \( d_f = 2 \), which is close to our estimation Eq. (12).

Interestingly, the similar spatially heterogeneous structures are observed for super-cooled liquids near the glass transition point \[39\]. For the studies of the glass transition, the degree of spatial heterogeneity is characterized by the so-called non-gaussian parameter \[40, 41\]. In our setting, an analogous quantity may be written as

\[ \alpha_2 = \frac{3 \langle (\delta \varphi^{2N^A})^4 \rangle}{5 \langle (\delta \varphi^{2N^A})^2 \rangle^2} - 1 = \frac{3}{5P} - 1. \] (13)

If the displacements follow the featureless gaussian distribution, one obtains \( \alpha_2 = 0 \). For the supercooled liquids, \( \alpha_2 \) of the displacements during the relaxation time rapidly increases on decreasing the temperature \[41, 42\]. Similarly, \( \alpha_2 \) of our model increases on approaching \( \varphi_f \), because \( P \to 0 \) and \( \alpha_2 \propto P^{-1} \). Furthermore, an experimental study for the supercooled colloidal suspensions, which approximately behave as hard spheres \[43, 44\] and may have the same interaction as our model below jamming, showed that the dynamically correlated regions form a compact cluster of the fractal dimension \( d_f = 1.9 \pm 0.4 \) \[42\], reasonably close to our result Eq. (12).

These results suggest the existence of the underlying universality between the dynamics of the athermal system near \( \varphi_f \) and thermal systems near the glass transition point \[45, 46\].

FIG. 2. Spatial distribution of non-affine displacements for \( N = 4092 \) particles. Diameters of spheres represent the amplitude of the (normalized) non-affine displacements \( |e_i| \).

FIG. 3. (a) Participation ratio \( P \) in \( d = 3 \). Markers denote numerical results, and solid lines are a guide to the eye. (b) Scaling plot of the same data.
Distribution function—

By using

\[ e_i \cdot e_i = \Delta_i \frac{3\delta^2}{\sum_1^N (\delta_i^4)^2} \]  

(14)

one can rewrite \( P \) as

\[ P = \langle \Delta \rangle^2 \]  

(15)

where

\[ \langle \Delta^n \rangle = \frac{1}{N} \sum_{i=1}^N \Delta_i^n = \int_0^\infty d\Delta f(\Delta) \Delta^n, \]  

(16)

with

\[ f(\Delta) = \frac{1}{N} \sum_{i=1}^N \delta(\Delta - \Delta_i). \]  

(17)

Here, we discuss the behavior of \( P \) from the perspective of the distribution function \( f(\Delta) \) near \( \varphi_J \). Fig. 4(a) presents \( f(\Delta) \) for several \( \delta \). \( f(\Delta) \) has a broader distribution for smaller \( \delta \). For the later convenience, we define a scaled variable \( x = \Delta/\langle \Delta \rangle \), and distribution function

\[ F(x) = f(\Delta) \frac{d\Delta}{dx} = \langle \Delta \rangle f(\langle \Delta \rangle x). \]  

(18)

By definition, \( \int dx F(x) = \int dx F(x)x = 1 \). As shown in Fig. 4(b), with decreasing \( \delta \), \( F(x) \) develops the power-law tail

\[ \lim_{\delta \phi \to 0} F(x) \sim x^{-\zeta} \text{ for } x \gg 1. \]  

(19)

A similar fat-tail was previously reported for the velocity distribution of sheared driven systems in the quasi-static limit near \( \varphi_J \). Now, we show that the exponent \( \zeta \) relates to \( \gamma \) in Eq. (11). First, using Eqs. (15)-(16), and (18), we get

\[ P = \left( \int_0^\infty dx x^2 F(x) \right)^{-1}. \]  

(20)

If \( \zeta < 3 \), the denominator diverges, leading to \( P = 0 \) at \( \varphi_J \). For finite \( N \), however, the divergences does not occur as the power law of \( F(x) \) is truncated at finite \( x_{\text{max}} \). Using the extreme value statistics, we can calculate \( x_{\text{max}} \) as

\[ \int_0^{x_{\text{max}}} F(x) dx \sim \frac{1}{N} \to x_{\text{max}} \sim N^{\frac{1}{\zeta-1}}. \]  

(21)

Then, \( P \) for finite \( N \) is expressed as

\[ P \sim \left( \int_0^{x_{\text{max}}} dx x^2 F(x) \right)^{-1} \sim N^{-\frac{3-\zeta}{\zeta-1}}. \]  

(22)

Comparing this with Eq. (11) for \( \delta \phi = 0 \), we finally get

\[ \zeta = \frac{3 + \gamma}{1 + \gamma} - 2.57. \]  

(23)

This is consistent with the assumption \( \zeta < 3 \) and well agrees with the numerical result, see Fig. 4.

**Two dimensional system.**—Finally, we discuss the dimensional dependence of the critical exponent. We perform numerical simulations in \( d = 2 \) with the same interaction potential of Eq. (1). Fig. 5 shows the \( \delta \phi \) dependence of \( \langle \Delta \rangle \) in \( d = 2 \), where the numerical data are well fitted with \( \langle \Delta \rangle \sim \delta \phi^{-1.9} \). A similar but a slightly larger exponent \( \langle \Delta \rangle \sim \varphi^{-2.2} \) has been reported for a two dimensional system driven by the quasi-static shear. The value of the exponent in \( d = 2 \) is significantly different from that obtained in \( d = 3 \). The similar dimensional dependence of the critical exponents was previously reported for the shear viscosity and relaxation time below \( \varphi_J \).

**Summary and discussions.**—In summary, we investigated the statistical properties of the non-affine displacements below the jamming transition point. We showed

![FIG. 4. (a) Distribution of \( \Delta \) for \( N = 4096 \) in \( d = 3 \). Markers are numerical results, while the dashed line denotes the power law \( f(\Delta) \sim \Delta^{-2.57} \). (b) Distribution of \( x = \Delta/\langle \Delta \rangle \) for the same data. The dashed line denotes \( F(x) \sim x^{-2.57} \).](image)

![FIG. 5. \( \delta \phi \) dependence of \( \Delta \) in \( d = 2 \). Markers denote numerical results. The solid line denotes the power-law fit with \( \Delta \sim \delta \phi^{-1.9} \). For a comparison, we also show the power law in \( d = 3 \), \( \Delta \sim \delta \phi^{-2.5} \), with the dashed line.](image)
that the mean squared of the non-affine displacement diverges toward the jamming transition point. At the jamming transition point, the distribution of the non-affine displacements has a power-law tail, which induces the vanishing behavior of the participation ratio at the jamming transition point in the thermodynamic limit. We also found that the critical exponents in two and three dimensional systems are different, implying that the upper critical dimension is $d_{uc} > 2$, in contrast with above jamming where $d_{uc} \leq 2$.

An interesting question is how the present work relates to the previous works for the shear driven systems. As the shear viscosity $\eta$ diverges with the same critical exponent as the bulk viscosity $\eta_p$ near $\varphi_f$ \cite{51,52}, we consider a system compressed with a finite compression rate $l = L/L_i$, instead of the shear driven system. The work done by the imposed compression per time is $p l L^3 = \eta_p l^2 L^3$, where $p$ denotes the pressure, and $\eta_p = p/l$ denotes the bulk viscosity. In the quasi-static limit $l \to 0$, this should be balanced with the dissipation $\sum_{i=1}^{N} \left( \frac{\delta x_i^{NA}}{l} \right)^2$, leading to \cite{28,53}

$$\eta_p \sim \frac{1}{L^3} \sum_{i=1}^{N} \left( \frac{x_i^{NA}}{l} \right)^2 \sim \frac{1}{L^3} \sum_{i=1}^{N} \left( \frac{\delta x_i^{NA}}{\delta l} \right)^2 \sim \langle \Delta \rangle. \tag{24}$$

A recent numerical simulation of a sheared suspension in $d = 3$ shows $\eta \sim \eta_p \sim \delta \varphi^{-\beta'}$ with $\beta' = 2.55$ \cite{29}, which is close to our result $\langle \Delta \rangle \sim \delta \varphi^{-\beta'}$ with $\beta = 2.5$ and thus agrees with the above conjecture. However, a more recent work reported a different value $\beta' = 3.82$ \cite{54}. Further theoretical, numerical, and hopefully experimental studies are necessary to elucidate this point.

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