Response of Granular Materials to Shear: Origins of Shear Jamming, Particle Dynamics, and Effects of Particle Properties

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Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Department of Physics in the Graduate School of Duke University 2018
Abstract

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Abstract

Granular materials under shear are common in nature and industry. Previous results show changes of system behaviors when friction is added and particle shapes are varied, e.g. shear jamming for frictional grains. Understanding these changes depends on characterization of deformation induced by shear. However, previous studies mainly focus on yielding processes and are locally symmetric, e.g. shear transformation zones (STZ’s). Besides, the grain scale explanation is lacking. In this thesis, I study the shear response of granular materials with various particle properties in two dimension, utilizing a novel setup that suppresses shear banding. Particles made of photoelastic materials can reveal inter-particle contact forces and be customized to have different friction and shapes. I propose novel minimum structures, trimers and branches, that account for shear jamming. These structures are locally asymmetric, which is contrary to STZ’s. Systems with three different friction coefficients $\mu$ are studied: 0.15, 0.7 and one higher than 1.7. Shear jamming is still observed for the lowest $\mu$ studied, with the lowest value of packing fraction $\phi$ for shear jamming, $\phi_S$, increasing as $\mu$ decreases. Furthermore, these systems for all $\mu$ show abnormal diffusion under cyclic shear. The diffusion exponents show transitions as $\phi$ increases, with a $\mu$-dependent onset $\phi$. This behavior is consistent with the non-affine displacements under linear shear. In addition, systems composed of ellipses exhibit novel structural and mechanical responses different from disks, e.g., nematic ordering and local density variability under shear.
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List of Abbreviations and Symbols

Symbols

All symbols below are also defined in the main text where they first appear.

- \( \phi \): Packing fraction of a collection of granular particles in a cell, defined as the total area of particles divided by the total area of the cell in 2 dimension.
- \( \phi_J \): The isotropic jamming point.
- \( \phi_S \): The lowest packing fraction for a system for shear jamming to happen.
- \( \tau \): Shear Stress.
- \( \sigma \): Stress tensor.
- \( \gamma \): Shear strain.
- \( C \): Fabric tensor.
- \( P \): Pressure.
- \( \mu \): Inter-particle friction coefficient.
- \( O \): The geometric measurement of a trimer incorporating its bending angle and its orientation relative to the compression direction of shear.
- \( \alpha_D \): The diffusion exponent of the mean squared displacement.
- \( \alpha_R \): The diffusion exponent of the mean squared rotation.
- \( \theta_e \): The orientation of an ellipse.
- \( Q \): Nematic matrix.
\( S \)  
Nematic order determined from the nematic matrix.

\( \theta_{ep} \)  
The preferred orientation determined from the nematic matrix.

**Abbreviations**

SJ  
Shear jamming.

MSD  
Mean squared displacement.

MSR  
Mean squared rotation.
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1

Introduction

1.1 Granular Materials

Granular materials are common. From a box of cereal (Fig. 1.1(a)), to a pile of fruit, to many industrial processes like transportation of ores and making of pills (Fig. 1.1(b)), to sand on the beach or in an hourglass (Fig. 1.1(c)), to soils and rocks all around us (Fig. 1.1(d)), these materials, which have a huge impact on our daily life, are granular materials from a physics perspective. Granular materials are composed of macroscopic particles that interact with each other via contact forces, which are usually frictional. These materials are a-thermal systems because the thermal energy \(k_B T \approx 10^{-21} \text{ J for room temperature } T \approx 300 \text{ K}\) is exceedingly small compared to even low kinetic energy \(10^{-12} \text{ J for a sand grain with a mass of 1 mg and a velocity of 1 mm/s}\) to allow systems to explore the phase space.

Granular materials show striking phenomena that have attracted research interests from a broad variety of fields, including mathematics, physics, engineering and biology. Take the sand in an hourglass as an example. Right after sand grains pass through the opening, they are separated and dilute, similar to a gas-like state.
Figure 1.1: Examples of granular materials: (a) cereal, (b) pills in a pharmaceutical production line, (c) sand in an hourglass, and (d) rocks and soils that fail in a landslide.

When they fall on the bottom of the hourglass, they interact with each other and the bottom, flowing like a liquid before they come to a stop due to inelastic collisions and frictional dissipation. At the end, sand grains form a mechanically stable heap, behaving like a solid. This typical example shows the rich behavior of granular materials under various conditions. The dissipative interactions distinguish granular materials from other thermal systems.

For instance, granular system that behave like liquids are common in many industrial processes such as transport in chutes, tumbler mixer and natural disasters
such as landslides. Efforts have been made to understand this flow. For instance, Boyer et al. has proposed a dimensionless number $I$ to unify suspension and granular rheology [1]. The inertial number $I$ is defined as $I = d\sqrt{\rho/P\dot{\gamma}}$, where $d$ is the average particle diameter, $\rho$ is the material density, $P$ is the system pressure, and $\dot{\gamma}$ is the shear rate. Then the system-wide friction coefficient $\mu$, defined as the shear stress divided by pressure, depends phenomenologically only on $I$. This analysis is called $\mu(I)$ rheology. The $\mu(I)$ description has been applied widely to describe dense suspensions and granular flows [2, 3, 4, 5, 6]. However, this analysis assumes the system is homogeneous and thus lacks microscopic insight to explain the origins of the flow behavior. Another approach providing a smaller scale yet continuous description is coarse-graining [7, 8]. In this approach, grain-scale properties are smoothed with a Gaussian or other functions $f(\mathbf{r} - \mathbf{r}_i(t))$ with a width $w$. Then the density field is given by $\rho(\mathbf{r}, t) = \sum_i m_i f(\mathbf{r} - \mathbf{r}_i(t))$. Furthermore, the velocity field can be defined as $v(\mathbf{r}, t) = p(\mathbf{r}, t)/\rho(\mathbf{r}, t)$, with the momentum field given by $p(\mathbf{r}, t) = \sum_i m_i v_i f(\mathbf{r} - \mathbf{r}_i(t))$. The coarse-graining approach has proven powerful and effective in two dimensional granular flows [9, 10]. However, this approach requires the acquisition of particle positions at all times, which poses difficulty in three dimensional situations and flows that are too fast for equipment to record.

Studying granular materials is not just of academic interest. By having a deeper understanding of them, we can design and engineer materials that exhibit special properties that are otherwise inaccessible. For instance, Fig. 1.2(a) shows a robot gripper that utilizes different phases of a granular system [11]. The gripper consists of granular materials confined in a soft rubber bag, which is connected to a vacuum machine. When the bag is inflated, the material can flow like a liquid, providing an adaptive way to surround objects of various shapes. Then the bag is evacuated, causing the gripper to behave like a solid and thus to be able to hold the object firmly. Interestingly, though little is understood about this liquid-like to solid-like
Figure 1.2: Sample applications of granular materials. (a) A robot gripper consisting of a soft rubber with granular materials enclosed. By changing the amount of air in the bag, the gripper can flow around an object with any shape and then become solid to hold the object. Figure adapted from [11]. (b) A reshapable toy called Vac-Man using a similar method as in (a), which came on the market in the 1990s. (c) Star-shape like particles that can form a mechanically stable structure without adhesion, providing solutions to programable architecture materials with the capability to be recycled. Figure adapted from [12].

transition, Cap Toys applied a similar method to make a toy called Vac-Man in the 1990s, whose body could be shaped and stay strong after the air was sucked out, e.g. Fig. 1.2(b). Fig. 1.2(c) shows another example where architects can construct a stable and strong structure just by changing particle shapes, e.g. from convex to non-convex shapes, without adhesion [12, 13, 14]. These particles can potentially serve as reusable architectural materials, allowing recycling instead of destroying of materials. From these examples, we see that studying granular materials is not
Phase diagram for amorphous systems, including granular matter, colloids, and glass forming materials. In this phase diagram, three parameters determine the state of materials: packing fraction or density, stress, and temperature. Granular materials, being a-thermal, live in the density-stress plane. A system can be in either jammed or unjammed state, as illustrated in this hypothetical phase diagram. Of particular interest is a point on the density axis, denoted as point J, close to which systems are critical. Figure adapted from [15].

only of great theoretical interest but also of great potential for daily and industrial applications. In this thesis, I will only focus on the static or quasi-static properties of granular materials, mainly dealing with the solid state and transitions from liquid-like to solid-like states.

1.2 Jamming

1.2.1 Isotropic Jamming

For static packings of granular materials, Liu and Nagel proposed a phase diagram to describe their mechanical stability, as shown in Fig. 1.3 [15, 16]. This phase diagram
incorporates not only granular materials but also other amorphous materials such as foams, colloids, glass forming materials and so on. A system can be in a jammed state, i.e. solid-like, or a unjammed state, i.e. liquid-like or gas-like, as determined by three control parameters: packing fraction ($\phi$) or density, applied stress ($\tau$) and temperature ($T$). Granular materials are a-thermal, therefore only controlled by packing fraction and applied stress. On the packing fraction axis, there exists a point of particular interest that shows critical behavior, referred as point J. And the corresponding packing fraction is named $\phi_J$.

One criterion to determine whether a system is isotropically jammed or not is the average contact number, $Z$. According to the Maxwell isostaticity argument, the number of contact forces must be equal to or greater than the degrees of freedom to have a mechanically stable system [17]. In the case of $N$ round rigid frictionless particles in $d$ dimension, the degrees of freedom is $Nd$ and the number of unknown forces is $NZ/2$ because only the magnitude of the contact forces can be varied. This reveals $Z_c = 2d$ at the isotropic jamming point J. If the particles are frictional, then the number of degrees of freedom become $Nd(d+1)/2$ because particle rotations need to be taken into consideration and the number of unknown forces becomes $NZd/2$. This gives $Z_c = d + 1$ for (very high) frictional particles. In the case of particles with irregular shapes, e.g. ellipses, this calculation still holds for frictional particles. However, for frictionless particles, the degree of freedom increases to $Nd(d+1)/2$, resulting in $Z_c = d(d + 1)$. Note that the Maxwell argument changes for finite friction. If the number of contacts at the point of friction failure is significant, then $d + 1 \leq Z_{iso} \leq 2d$.

By simulating a-thermal soft frictionless granular systems under isotropic conditions, i.e. zero applied shear stress, O’Hern et al. found $\phi_J \approx 0.84$ in 2D and
\( \phi_J \approx 0.64 \) in 3D [18]. In this simulation method, particles interact via a potential:

\[
V(r_{ij}) = \Theta(1 - \frac{r_{ij}}{\sigma_{ij}}) \cdot \frac{\epsilon}{\alpha}(1 - \frac{r_{ij}}{\sigma_{ij}})^\alpha,
\]

where \( r_{ij} \) is the distance between particles \( i \) and \( j \), \( \epsilon \) sets the energy scale of the interaction, \( \sigma_{ij} \) is the average of the diameters of particles \( i \) and \( j \), and \( \Theta \) is the Heaviside function. \( \alpha = 2 \) and \( \alpha = 5/2 \) correspond to harmonic and Hertzian repulsive forces, respectively. Simulations show the emergence of non-zero average contact number \( Z \), pressure \( P \), shear modulus \( G \), and bulk modulus \( B \), as \( \phi > \phi_J \).

For instance, at \( \phi = \phi_J^- \), there are no particles in contact, i.e. \( Z = 0 \), while for \( \phi = \phi_J^+ \), \( Z \) jumps to \( Z_c \) discontinuously.

Point J shows critical scaling behavior for a number of quantities as a function of \( \Delta \phi = \phi - \phi_J \), the distance to \( \phi_J \) from above [18, 15, 19]. The excess number of contacts scales as \( \Delta Z = Z - Z_c \sim \Delta \phi^\beta \) with \( \beta \approx 0.5 \). Pressure scales as \( P \sim \Delta \phi^\psi \), with \( \psi \approx 1 \) for \( \alpha = 2 \) and \( \psi \approx 1.5 \) for \( \alpha = 5/2 \). The shear modulus scales as \( G \sim \Delta \phi^\gamma \), with \( \gamma \approx 0.5 \) for \( \alpha = 2 \) and \( \gamma \approx 1 \) for \( \alpha = 5/2 \). The ratio of the shear modulus to the bulk modulus scales as \( G/B \sim \Delta \phi^\nu \) with \( \nu \approx 0.5 \). That is, \( G/B \) scales as \( \Delta Z \) for frictionless particles. In addition, the pair correlation function, \( g(r) \), which measures the probability of finding a particle at \( r \) given one at the origin, shows a divergent first peak at point J. The first peak value, \( g(r_0) \), diverges as \( \Delta \phi \) decreases: \( g(r_0) \sim \Delta \phi^{-1} \). The width of the first peak, or the overlap distance, \( l_w \), vanishes with \( \Delta \phi \) as \( l_w \sim \Delta \phi \). In addition, a study of the rheology of systems close to jamming also suggests the criticality of point J [20]. In this study, the viscosity, defined as the steady-state shear stress over the shear rate, shows scaling collapse onto two branches, one above and the other below the isotropic jamming point \( \phi_J \).

The critical behavior exhibited at the jamming transition has also been seen in several models, such as those that capture glassy dynamics [21, 22, 23, 24, 25] and those related to percolation [26, 27, 28, 29, 30].
1.2.2 Shear Jamming

Results summarized above in Sec. 1.2.1 are obtained from frictionless granular systems. For frictional systems, Silbert has shown that the isotropic jamming point increases as the friction coefficient $\mu$ decreases, along with a $\mu$-dependent $Z_{iso}$ [31]. These values approach to the ones in the frictionless case as $\mu$ decreases. Meanwhile, there have also been experiments that generate highly anisotropic mechanical stable states, with a $\phi$ lower than $\phi_J$ [32, 33, 34]. All these findings indicate differences between frictionless and frictional granular systems.

Bi et al. proposed new phases for frictional granular grains based on experiments in $2D$ [35]. The new phase diagram for frictional granular materials is depicted in Fig. 1.4(b). Their study has shown that systems below their isotropic jamming point ($\phi_J$) can develop mechanically stable force networks that percolate through the system, namely in jammed states, under quasi-static shear. This phenomenon of inducing jammed states by shear in a system with $\phi$ below $\phi_J$ is called shear jamming. Before the frictional system reaches shear jammed states from a stress free state, there also exists another state at which force networks form mainly in the compression direction of shear. Such a state are mechanically stable due to friction, however unable to sustain shear in the reversed direction. This special state has an average contact number less than the value needed for isotropic jamming and is referred as a fragile state [36]. In addition to the critical point $\phi_J$, there also exists another important point, namely the lowest $\phi$, below which shear jamming cannot happen. This point is denoted as $\phi_S$.

Shear jamming in a conserved area/volume, presumably shares a similar origin with shear dilatancy in systems with deformable boundaries. Shear dilatancy was first observed by Osborne Reynolds in 1885, when he showed that a packing of frictional grains would expand under shear if they were confined at fixed pressure [37].
FIGURE 1.4: (a) Original Liu-Nagel phase diagram for frictionless granular materials, which is the $T = 0$ plane in Fig. 1.3. In this phase diagram, $\phi$ is the packing fraction and $\tau$ is the shear stress. (b) Generalized phase diagram for frictional granular materials. Compared to the original Liu-Nagel phase diagram, a granular system can be in new phases, namely shear jammed (SJ) and fragile (F) states, even when its $\phi$ is below $\phi_J$. There exists a lowest $\phi$, below which shear jamming cannot happen, denoted as $\phi_S$. Figures adapted from [35].

Whether shear jamming and shear dilatancy exists in frictionless systems remains under debate. Roux and Radjai showed that frictionless systems did not macroscopically dilate under shear [38], although Imole et al. reported some volumetric response, depending on initial conditions [39]. Other recent work has shown that shear jamming features occur for frictionless particles [40, 41]. Baity-Jesi et al. have shown that the shear jamming range of $\phi$, i.e. $\phi_J - \phi_S$, vanishes as the system size grows [42], unlike for the frictional case where shear jamming occurs for a non-zero range of $\phi$’s for large systems [35, 43].

Since the concept of shear jamming has been introduced, it has attracted much research attention. People have found that shear jamming extends beyond static granular materials; it has been reported in other systems and processes, such as suspensions [44, 45, 46], granular impacts [47] and flow [48]. For instance, discontinuous shear thickening (DST) has been found in many non-Newtonian suspensions including cornstarch-water mixtures [49]: the shear viscosity increases with shear rate and
such an increase is discontinuous at a certain shear rate. One of the widely accepted theories accounting for DST is to include both relevant frictionless hydrodynamic interactions and frictional contacts: at low shear rate, the hydrodynamic interactions dominate and provide lubrication between suspended particles; at high shear rate, particles start to make frictional contacts and a high viscosity results from the shear jammed states [44, 46]. This type of granularlike contact has recently been validated by Corntet et al. [50].

1.3 Yielding, Failure and Plastic Deformation

Granular materials deform when they undergo compression or shear, processes which are common in many natural and industrial processes. If the strain/stress is small, the system can sustain the applied stress and deform elastically. For a large enough strain/stress, the system fails or yields with regions undergoing plastic deformation. For example, a packing of granular pillars are compressed under a small constant speed $v_c$ without constraints in the horizontal direction (Fig. 1.5(a)). Instead of expanding uniformly like a bulk of elastic material does, the pillars display velocity gradients as their distance to the compression panel increases, with regions showing sharp change of particle velocities, as shown in Fig. 1.5(b). These regions correspond to yielding and their deformation is plastic, i.e. irreversible. There have been a lot of methods to describe yielding and plastic deformation [51, 52, 53]. In this section, I will introduce two widely used approaches.

1.3.1 Mohr-Coulomb Failure Analysis

In the Mohr-Coulomb failure analysis, granular materials are modeled as an ideal Coulomb material [51]. A rigid-plastic failure mode is assumed, in which materials are divided into rigid blocks separated by narrow plastic zones during yielding. For the ideal Coulomb material, the pressure $P$ and the shear stress $\tau$ applied on
the plastic zone is assumed to take a linear form as the Coulomb yield criterion:
\[ \tau = \mu P + c \]
where \( \mu \) and \( c \) are the coefficient of friction and the cohesion of the materials, respectively. The Coulomb yield criterion is further combined with the Mohr circle, whose center \((p, 0)\) is the system’s pressure and the radius is determined by a combination of components of the stress tensor [51], to show all allowed states of \((P, \tau)\) without material yielding.

Fig. 1.6 illustrates the Mohr-Coulomb failure analysis. Different situations are plotted in line (i), (ii), and (iii). If the system lives on line (i), then \( \tau < \mu P + c \). According to the Coulomb criterion, this state is stable and no yielding occurs. Line (ii) is tangent to the Mohr circle, indicating \( \tau = \mu P + c \). If the system is along this line, then yielding is about to happen at the point of tangency. Line (iii) cuts through the Mohr circle and hence indicates the existence of states \( \tau > \mu P + c \), which are forbidden. One thing to note is that the failure process does not depend on the sign of \( \tau \). Hence the above analysis still holds if the above lines are symmetric about the \( P \) axis. The Mohr-Coulomb analysis also reveals the angle between the slip plane and the minor axis to be \( 45^\circ - \theta \), where \( \theta \) is given by \( \tan \theta = \mu \).

This model assumes that the material is divided into two elastic parts with a
Figure 1.6: An illustration for the Mohr circle analysis for material failure, where $P$ is pressure and $\tau$ is shear stress. Line (i) indicates that all the possible states, i.e. all the points in the Mohr circle, satisfy $\tau < \mu P + c$, therefore the system is stable and no slip zone will occur. Line (ii) stands for the Coulomb yield line, where at point of tangency to the Mohr circle: $\tau = \mu P + c = P \tan \theta + c$. If the system lives on line (iii), then it is unstable and yields.

narrow slip zone between. This predicts the onset of yielding. However, being a dynamic process, yielding changes over time and the slip zone may have an effect on the elastic parts. In addition, yielding may happen as well in the elastic parts, with smaller amplitude. Therefore, a more realistic model taking smaller scales into account is needed. Though over-simplified, the Mohr-Coulomb analysis has been applied widely for commercial purposes and forms the basis of a number of other more accurate models, such as the Conical yield function [51] and the critical state soil mechanics [55, 56].

1.3.2 Shear Transformation Zones

Falk and Langer proposed a different approach to quantify deformation locally, called $D_{min}^2$. In order to compute the local strain for each grain, neighbors that are close enough to this grain, usually within the interaction range, are included and assumed
to be in a region of uniform strain $\varepsilon_{ij}$. The following quantity is then defined:

$$D^2(t, \Delta t) = \sum_n \sum_i (r^i_n(t) - r^i_0(t)) - \sum_j (\delta_{ij} + \varepsilon_{ij}) \times [r^j_n(t - \Delta t) - r^j_0(t - \Delta t)])^2, \quad (1.2)$$

where $i$ and $j$ are the indices of spatial coordinates, $n$ is the index of particles in the region considered, $r^i_n(t)$ is the $i$th component of the position of the $n$th particle at time $t$. The local strain $\varepsilon_{ij}$ is then given by minimizing $D^2$, which involves computing the following quantities:

$$X_{ij} = \sum_n [r^i_n(t) - r^i_0(t)] \times [r^j_n(t - \Delta t) - r^j_0(t - \Delta t)], \quad (1.3)$$

$$Y_{ij} = \sum_n [r^i_n(t - \Delta t) - r^i_0(t - \Delta t)] \times [r^j_n(t - \Delta t) - r^j_0(t - \Delta t)], \quad (1.4)$$

$$\varepsilon_{ij} = \sum_k X_{ij} Y^{-1}_{jk} - \delta_{ij}. \quad (1.5)$$
The minimum value of $D^2$, denoted $D_{\text{min}}^2$, thus quantifies the local deviation from the affine strain during a given time interval.

A large $D_{\text{min}}^2$ corresponds to a region where plastic deformation happens. These regions are referred to as shear transformation zones (STZ’s). For instance, as shown in Fig. 1.7 highlighted by an oval, a group of one large and three small particles are compressed along one diagonal direction (top-left to bottom-right) and stretched in the perpendicular one with particles notably rearranged. Such a group of four particles forms a minimum STZ and the deformation of this group described above is usually called a T1 event. STZ’s have been applied widely and successfully to amorphous systems like metallic glass, colloids and granular materials to explain yielding and plastic deformation [57, 58, 59, 60, 61, 62].

Recent development in describing structure configuration and particle dynamics in plastic deformation and out-of-equilibrium glassy systems incorporates machine learning to define a quantity called softness [63, 64, 65]. Based on their structural configurations and a machine learning model, regions of particles with large softness are predicted to rearrange and deform plastically and softness is typically well correlated with the $D_{\text{min}}^2$ measurement in the STZ’s framework. Predictions based on softness show commonality for disordered packings of particles ranging from atom to granular grains, spanning seven orders of magnitude in diameter [64].

1.4 This Work

These studies and others show that sheared frictional systems are usually anisotropic and display different behaviors from frictionless systems. However, little is understood about the role of friction and other particle properties. In addition, most work done to explain the response of granular materials assumes an isotropic homogeneous system or are locally symmetric. But these assumptions may break down due to the anisotropy enabled by friction. The questions I seek to answer in this work are:
what is the microscopic, i.e. grain-scale, origin of shear jamming and how do particle properties affect the response of a granular system to shear? A recently developed experimental setup in the Behringer lab enables application of homogeneous shear to granular systems without generating shear bands. By using photoelastic materials, we access particle positions and orientations and inter-particle contact forces. The photoelastic materials also allow us to easily modify particle properties, such as particle shapes and inter-particle friction. In this study, I present results that bring novel insights to better understand the response of granular materials to shear and hence the nature of granular materials.

The remainder of this thesis is organized in the following way. In Chapter 2, I introduce the experimental setup along with the materials used, and general techniques to process raw data to obtain information of interest. In Chapter 3, I propose novel mechanisms accounting for shear jamming of frictional grains. In Chapter 4, I explore the effect of friction on shear jamming of systems with various friction. Their translational and rotational diffusion properties are studied in Chapter 5. In Chapter 6, I present response to shear of a granular system with an anisotropic shape, i.e. ellipses. The results and possible future directions are summarized in Chapter 7.
The approach to understanding the nature of granular materials in this thesis study is to apply shear with conserved area in two dimension (2D) using particles with various properties. Commonly used shear cells in 2D are wall-driven, with granular materials sitting on a base. One drawback with this type of driving mechanism is that because of basal friction particles are not carried smoothly by the shear profile, for instance, when they are far away from the sidewalls. This is especially true when the packing fraction is much lower than the jamming point. Associated with such an inhomogeneous shear profile are shear bands, where particles have relatively larger displacements and local packing fractions are lower than those out of shear bands. Though shear bands are inevitable in nature, they are unfavorable here because the system would be not uniform if they were to form.

In light of this issue with inhomogeneity, a new apparatus has been developed to suppress shear bands [43]. Friction between granular particles and the base still exists, however, this apparatus utilizes this specific friction to provide a homogeneous shear profile. In this chapter, I introduce the apparatus, granular particles used for experiments, the automatic control system, and general techniques applied to extract
information of interest from raw experiment data, i.e. digital images.

2.1 Experiment Setup

The experiment setup consists of three parts: a novel shear cell designed to provide homogeneous shear to a system of granular particles made of photoelastic materials, an optical system with a digital camera to acquire raw images, and a control system coordinating the tasks to apply a certain amount of shear deformation and to record experiment data.

The shear cell is mainly composed of four aluminum sidewalls in a parallelogram shape and 49 plexiglass slats forming the base, as shown in Fig. 2.1(a). The cell has a width of \( w = 29.7 \) cm and a length of \( l = 62.1 \) cm, and each slat is of width 1.26 cm. A stepper motor is connected to one of the sidewalls to shear the cell in the \( y \) direction (Fig. 2.1(a)). The slats are attached to the two longer sidewalls, yet can slide freely along those two walls so that the slats can maintain their \( x \) positions when the cell is sheared along the \( y \) direction, as in Fig. 2.1(a). Then the shear strain is defined as the deformation in the \( y \) direction over the length in the \( x \) direction, i.e. \( \gamma = \Delta y/l \).

Sitting on the slats are particles made of photoelastic materials, which under anisotropic stress will light up and show fringe patterns if placed between a pair of crossed polarizers. The first set of experiments are done with discs. Then another shape is investigated, i.e. ellipses. Any specific experiment uses only one type of shape, and no mixture of different shapes are studied. Particles are cut by machine or thin water jet from photoelastic sheets (Vishay PSM-4) of height 0.64 cm. The material has a Young's modulus of about 4 MPa. Another photoelastic material (Precision Urethane with a Young’s modulus of approximately 4 MPa) is also used to produce extremely large friction particles and particles with larger sizes than the ones initially investigated. Particle dimensions will be listed throughout the text.
Figure 2.1: A sketch for the experimental setup. (a) A top view of the shear cell. When the sidewalls deform to create simple shear, the slats move with the walls so that the base deforms affinely. In the sketch, both the slats and particles are drawn much larger relative to the boundaries than in the real experiment. The $x-y$ axes indicate the coordinate system in the lab frame, where simple shear is applied along the $y$ axis, and the shear strain, $\gamma$, is defined as $\gamma = \Delta y / l$. (b) A side view of the optical system, with the shear cell included. The shear cell and particles are put between a pair of circular polarizers, which consist of a linear polarizer and a quarter-wave plate. The polarizer in front of the camera is moved by a stepper motor into or out of the scope of the camera.
To maximize the information that can be obtained from these photoelastic particles, three kinds of pictures are taken under different light conditions with a high-resolution camera (Canon 5D Mark II, $3744 \times 5616$ pixels). A sketch of the optical system can be found in Fig. 2.1(b). Two types of light sources are used: white light and UV light. When the white light is on, the UV light is off. And vice versa. The white light goes through a circular polarizer, which shifts the phase of a green light with a $560 \, \text{nm}$ wavelength by $\pi/4$, and then through the photoelastic particles. Before this light reaches the camera, another piece of circular polarizer can be placed either in ('P' image) or out ('N' image) of the view of the camera, which is done with a stepper motor. ‘N’ and ‘P’ images can be used to determine particle centers and contact forces, respectively. When the white light is off, UV light can excite an UV ink bar plotted roughly at the center of each particle, which is invisible under normal light condition. These bars indicate particle orientations. Such an image is referred as a ‘U’ image. Examples of these three kinds of images can be found in Fig. 2.2.

Shear experiments are carried out quasi-statically. For any experiment, the sys-
FIGURE 2.3: A schematic sketch of the circuit connected to Raspberry Pi (R-Pi) for controlling the experimental setup. Lines with different types and colors indicate wires. Numbers indicate different pins controlled by R-Pi as either inputs or outputs, depending on the actual use. Here, 12 and 25 are used as inputs and the rest are outputs. Two stepper motors are connected to R-Pi. One of them drives the shear cell with a certain speed and distance indicated by R-Pi from pins 6, 13, and 19, and the other is controlled by pins 5, 22, and 27 to move the polarizer in front of the camera. The camera is connected to R-Pi via a USB connection, commanded to take pictures with a required exposure time and ISO value by the library ‘gphoto2’. Both white light and UV light can be switched on or off by controlling relays connected to them. Two limit switches are constantly checked by R-Pi to prevent over-deforming the shear cell caused by malfunction or mistakes.

The system is deformed by a small amount of shear strain, typically $\delta \gamma = 0.0027$, followed by letting the system relax for 6 seconds and then taking three kinds of pictures (‘N’, ‘P’ and ‘U’). Such a process of shear, relaxing and picture taking is repeated until a certain shear strain is achieved. Two kinds of shear are investigated in this study: shear in one direction with a relatively large shear strain (referred as linear shear) and shear back and forth in small deformation (referred as cyclic shear). For linear...
shear, quasi-static shear is repeated multiple times to achieve a shear strain up to
\( \gamma = 0.54 \), which is the maximum shear strain allowed for this setup. For cyclic shear,
the system is sheared in one direction by a few steps till a maximum value is reached
for the shear strain \( \gamma = \gamma_{max} \), then the shear direction is reversed and the system is
sheared by the same amount of steps. For experiments performed in this work, \( \gamma_{max} \)
is relatively small, usually a few percent. Cyclic shear with multiple cycles can be
applied to mimic vibration or external activation.

In order to coordinate shearing with a certain step size and taking pictures af-
therwards, the optical system and the driving stepper motor are all connected to
Raspberry Pi (R-Pi), as shown schematically in Fig. 2.3. The R-Pi uses python
codes to control its pins, which can be used as either inputs or outputs, depending
on the actual case. The pins can control the on and off of the light sources via relays,
on/off, directions, and speeds of motors. The motor is driven by sending a series of
high and low voltage pulses from the R-Pi. The python codes can also command the
camera via a USB connection by using the library ‘gphoto2’, specifying the exposure
time, ISO value and aperture number. A typical shear step follows the procedure as
listed below, which is completely controlled by R-Pi:

1. The shear stepper motor (motor 1) is turned on to drive the system under a
certain constant speed for a certain distance and then stops.

2. After 6 seconds, the white light is turned on and then a ‘P’ image is taken with
a pair of crossed polarizers.

3. Another stepper motor (motor 2), which is connected to the piece of polarizer
right in front of the camera, is turned on to remove this polarizer from the
scope of the camera, after which an ‘N’ image is taken.

4. The white light is turned off and the UV light is turned on, then a ‘U’ image
is taken.

5. The polarizer is returned to its original place by motor 2 and the UV light is turned off.

Such a procedure is used as a building block in python to design more complex shear profiles, such as linear shear and cyclic shear.

2.2 Data Processing

2.2.1 Particle Tracking

From ‘N’ and ‘U’ images, I track centers and orientations of particles. For discs, Fig. 2.4 shows example images illustrating the process of finding centers and sizes of particles, i.e. circles, from the ‘N’ image. This process can be summarized as follows:

1. From the blue channel of the ‘N’ image, e.g. Fig. 2.4(a), a mapping of the intensities to new values by suppressing low and high intensities is employed to increase the contrast of the image.

![Figure 2.4](image-url)

**Figure 2.4**: An example showing the process of finding particle centers. (a) The blue channel of the same image shown in Fig. 2.2(a). (b) The result after increasing the image contrast and applying a low-pass filter to the Fourier transform of (a). (c) Detected discs with the blue circles indicating centers and radii of the particles.
2. Then a low-pass filter is applied to the Fourier transform of the image to remove straight lines caused by the edges of slats, especially for the edges passing through particles in the image. Fig. 2.4(b) shows the result after enhancing the contrast and removing lines inside of the particles.

3. Finally a circular Hough transform is applied to the gray scale image in Fig. 2.4(b) to find centers and diameters of the discs [66]. The transform is an algorithm computing the curvature at each pixel point based on the image gray scale gradient. The curvature will automatically give the center and radius. Then a voting process rules out fake circles and combines circles with close enough centers and similar radii. The final result of particle identification is shown in Fig. 2.4(c), where blue circles indicate particle centers and radii given by the algorithm with errors smaller than 0.02 times the particle diameter.

With the particle positions and radii information, orientations can be found in the ‘U’ image. Using the blue channel of the ‘U’ image, e.g. Fig. 2.5(a), an adaptive threshold is applied locally to binarize the image so that the UV bars are 1 and

![Figure 2.5](image)

**Figure 2.5**: An example showing the process of finding particle orientations. (a) The blue channel of the same image shown in Fig. 2.2(c). (b) The result after applying a locally adaptive threshold to binarize (a). (c) Detected particle orientations from the binary image in (b), with the red lines having the same orientation plotted at the center of particles.
Figure 2.6: Example images showing the photoelastic ellipse particles and the process to detect their centers and orientations. (a) Blue channel of a ‘U’ image, showing the UV bar (bright regions) drawn on each particle surface aligned with the major axis of the ellipse. (b) Green channel of a ‘N’ image. (c) Binarized image of (a), after a local threshold application to select all the UV bars (white areas). These bars can be identified by Matlab revealing centers and orientations, which provide a close estimate to information of particles associated by bars. (d) Particle edge detection from (b) after using the Sobel method. (e) An example of an ellipse edge mold rotated by 45° counterclockwise, which will be used to convolute with the actual particle edges, e.g. (d), provided the rough estimate results from (c). This mold has the same size as particles. (f) Final results of particle detection, shown as blue ellipses.

the rest of the particle is 0, as shown in Fig. 2.5(b). Then a least squares fit with the minimized perpendicular offsets reveals a linear function between the $x$ and $y$ positions in each UV bar, shown in Fig. 2.5(c). The slope of the line gives the orientation associated with each particle.

As for particles with an elliptical shape, another methods mainly involving convolution is used to detect particle center and orientation at the same time, combining ‘U’ and ‘N’ images, e.g. Fig. 2.6(a) and (b), respectively. Similar to discs, an invisible UV bar is also drawn at the surface of each ellipse. The bar is drawn in a special
way carefully, with the assistance of a 3D printed mold, so that the center of the bar coincide with the particle center and the direction of the bar is aligned with the major axis of the ellipse.

The same procedure as in the disc case is followed here to binarize the ‘U’ image so that UV bars can be separated from the rest of the image, with the result shown in Fig. 2.6(c). Each bulb, i.e. isolated white regions in the binarized ‘U’ image, can be detected in Matlab using function ‘regionprop’, which reveals the center and orientation of each bulb. This information, due to preparation of drawing UV bars, can be used as an rough estimate for particle centers and orientations. To accurately find particles, their edges are detected by the Sobel method, e.g. Fig. 2.6(d). Then a preset ellipse edge mold, whose orientation can be varied and size is the same as the particle, e.g. Fig. 2.6(e), is used to convolve with the detected edges. Convolution is done in 3 dimension \((x, y)\) positions and orientation) for each particle, with previous estimate information from the binarized ‘U’ image to reduce computation time. First a region centered at the estimated center with lengths approximately 20% larger than the major axis is selected. Then the ellipse edge molds with different orientations close to the estimated one are convolved with this region. Lastly the positions at the peak value of the convolution results gives the center and orientation. The final result of particle detection for Fig. 2.6(a) and (b) is shown in Fig. 2.6(f).

2.2.2 Contact Force

Once particle centers and radii are detected, it is possible to determine contact forces from the photoelastic response in the polarized image. The green channel of the image is used here because the quarterwave plate composing the circular polarizers works the best for 560 \(\lambda m\) light. There are two approaches available to be employed to reveal inter-particle forces: the squared gradient method and a nonlinear fitting algorithm to solve the vector forces, referred as \(G^2\) method and inverse algorithm in
the following of this thesis, respectively.

$G^2$ method computes the discrete squared gradient of the light intensity at each pixel point of the polarized image, defined as:

$$G^2(x, y) = \frac{1}{4}[I(x + 1, y) - I(x - 1, y)]^2 + \frac{1}{4}[I(x, y + 1) - I(x, y - 1)]^2$$

$$+ \frac{1}{8}[I(x + 1, y + 1) - I(x - 1, y - 1)]^2$$

$$+ \frac{1}{8}[I(x + 1, y - 1) - I(x - 1, y + 1)]^2,$$

where $I(x, y)$ is the intensity at the pixel position $(x, y)$. This definition takes into account the light intensity gradient in all four directions around pixel $(x, y)$, as illustrated in Fig. 2.7(a). An example showing the $G^2$ value at each pixel for the green channel of Fig. 2.2(b) can be found in Fig. 2.8(b), where $G^2$ is plotted logarithmically proportional to the color bar so that a broad range of $G^2$’s can be seen. It has been shown empirically that pressure is proportional to $G^2$ when averaged over all the pixel points in the region of interest, as shown in Fig. 2.7(c). This is generally valid for both a single particle and a collection of particles and is not sensitive to the shape of particles. The $G^2$ method, being able to reveal particle-scale pressure, provides

| (x-1, y-1) | (x-1, y) | (x, y) | (x+1, y) |
| (x, y-1) | (x, y) | (x+1, y) |
| (x+1, y-1) | (x+1, y) |

**Figure 2.7:** (a) An illustration for the pixels in an image and how $G^2$ is computed for pixel point $(x, y)$ by averaging in all the four directions (horizontal, vertical and two diagonal ones). (b) An image plotting pixel-wise $G^2$ values from the green channel of Fig. 2.2(b), in a logarithmic scale. (c) The empirical relationship between the applied pressure $P$ and $G^2$ averaged over the region of particles.
much more information than a force gauge, which can only measure the force acting on it, and is easily applied in a wide range of systems with different shapes. However, one drawback for $G^2$ method is that it cannot determine vector forces.

$G^2$ can also be used to help determine force-bearing contacts. Geometrically, if the distance between the centers of two circles are smaller than the sum of their radii, then these two circles intersect. However, such a criterion is not enough to determine whether a true force-bearing contact exists due to errors in detecting particle centers and radii and the nature of the contact force of elastic bodies (normally Hertzian). In order to correctly find contacts, firstly the distance between centers of two discs is compared with the sum of their radii. If this distance is smaller than a certain value, then $G^2$ is computed at the vicinity of the possible contact points, usually with a length of roughly $1/4$ diameter. Finally, if this $G^2$ passes a preset threshold, then a true force-bearing contact is determined. By applying the geometric and $G^2$ criteria for Fig. 2.8(a), contacts are determined, shown in Fig. 2.8(b) as crosses.

Once contacts are determined, the inverse algorithm, which employs a nonlinear fitting method, can solve the vector forces based on the property of the photoelastic material and elasticity of disc shape material with point contacts. For a sheet of photoelastic material, the transmitted light intensity $I$ at any image point is dependent on the phase shift $\alpha$ as the circular polarized light goes through the material: $I = I_0 \sin^2(\alpha/2)$. The shift is given by:

$$\alpha = \frac{2\pi C t}{\lambda} (\sigma_1 - \sigma_2), \quad (2.2)$$

where $C$ is the stress-optic constant for the material, $t$ is the thickness of the sheet, $\lambda$ is the light wavelength, and $\sigma_1$ and $\sigma_2$ are the two eigenvalues of the stress tensor. In terms of $\sigma_1 - \sigma_2$:

$$I = I_0 \sin^2\left(\frac{\pi C t}{\lambda} (\sigma_1 - \sigma_2)\right). \quad (2.3)$$
Figure 2.8: (a) The green channel of the same image shown in Fig. 2.2(b). (b) Detected contact positions for each particle with both the geometric and $G^2$ criteria satisfied, where contacts are marked as blue crosses. (c) Computed image intensity from the best fit contact forces for (a), using contacts information from (b) and the inverse algorithm. (d) The intensity difference between (a) and (c) to show a good fit between the actual intensities and the fitted ones, validating the robustness of the computed contact forces.

Hence, it is key to determine the difference between $\sigma_1$ and $\sigma_2$ once the sheet is chosen. However, it is impossible to find $\sigma_1 - \sigma_2$ just based on $I$ at a single point because a sin function is not a monotonic function. On the other hand, Majmudar et al. have shown that for an elastic disc bearing moderate point contact forces, the stress field at any point inside of the disc can be solved analytically by assuming negligible deformation at contact positions [67]. The stress field automatically reveals $\sigma_1 - \sigma_2$. Therefore, the force-solving problem becomes: how to solve $x$ given the value of $\sin x^2$? Such a problem falls into a category called the nonlinear inverse problem, which is to calculate the cause from the observation while the action from the cause to the observation is a nonlinear process. This kind of problem is generally hard to solve due to its nonlinearity nature.

In order to tackle this specific inverse problem here, an algorithm (the inverse
algorithm) was developed by Majmudar et al. [68] and later improved by Zhange et al. [35], given particle centers and sizes, contacts positions and the polarized image. A general flow of the algorithm is summarized as follows:

1. An initial guess for contact forces is given based on $G^2$ values averaged over the areas close to contacts, with force and torque balanced for each particle.

2. Areas with possible large intensity variance are chosen for calculating the artificial intensity given by the initial guess.

3. The difference between the artificial intensity and true intensity from the image is minimized by iteratively fitting contact forces using a nonlinear fitting algorithm (the Levenberg-Marquardt algorithm), while maintaining force and torque balance on the particles. When the minimum is reached, the best fit contact forces are obtained.

For discs, the inverse algorithm works fast and well, e.g. Fig 2.8(c), which calculates contact forces in Fig. 2.8(a) and plots the corresponding light intensity from these calculated forces. The robustness of the algorithm is further tested by subtracting Fig 2.8(c) from Fig. 2.8(a), shown in Fig. 2.8(d). However, so far this algorithm works well for disc shape so far because the stress field is known analytically in closed form for a circular boundary. It remains as a challenge to apply this method to other shapes, e.g. ellipses.

2.2.3 Fabric and Stress Tensors

Shear usually generates anisotropic contact and force networks. Commonly used methods to characterize anisotropy are to compute the fabric tensor and stress tensor, which are applicable at both the particle and the system scale.

Fig. 2.9(a) draws an example for one particle (particle 4) in contact with three other particles (1, 2 and 3) to help illustrate the definition of the fabric tensor and
stress tensor. Fig. 2.9(b) gives a sketch for the corresponding fabric and stress tensors eigenvalues, with arrows indicating the eigenvectors. It can be seen that the principal eigenvectors, i.e. the ones with larger eigenvalues, for fabric and stress tensors, do not necessarily align with each other. This is often the case for a force network of frictional particles induced by shear.

The fabric tensor for a particle is defined as:

$$C^{(k)} = \sum_l \frac{\vec{R}^{kl}}{R^{kl}} \otimes \frac{\vec{R}^{kl}}{R^{kl}} = \sum_l \frac{\vec{R}^{kl}}{R^{kl}} \cdot \frac{\vec{R}^{kl}}{R^{kl}},$$  \hspace{1cm} (2.4)$$

where \(k\) is the index of the particle being computed, \(l\) is the index of a particle in contact with \(k\), \(\vec{R}^{kl}\) is the vector from the center of \(k\) to the contact point between \(k\) and \(l\), and \(i\) and \(j\) are components of vectors in space. The system-wide fabric tensor for all the particles involved in the contact network can be computed by:

$$C = \frac{1}{N} \sum_k C^{(k)} = \frac{1}{N} \sum_{k,l} \frac{\vec{R}^{kl}}{R^{kl}} \otimes \frac{\vec{R}^{kl}}{R^{kl}}.$$  \hspace{1cm} (2.5)$$

where \(N\) is the total number of particles in the contact network. With two eigenvalues of \(C\) in 2D \((C_1\) and \(C_2\)), the fabric anisotropy is defined as \(|C_1 - C_2|/(C_1 + C_2)\).

The trace of \(C\), i.e. \(C_1 + C_2\), equals the average contact number per particle.

The stress tensor for a collection of particles is determined from the force moment tensor of each particle, which for particle \(k\) is defined as:

$$\Gamma^{(k)} = \sum_l \vec{R}^{kl} \otimes \vec{F}^{lk} = \sum_l R^{kl}_i \cdot F^{lk}_j,$$  \hspace{1cm} (2.6)$$

where \(\vec{F}^{kl}\) is the force acting from \(l\) to \(k\), and the rest symbols have the same meaning as in Eq. 2.4. Then the system-wide stress tensor for all the particles involved in the force network is calculated as:

$$\sigma = \frac{1}{A} \sum_k \Gamma^{(k)} = \frac{1}{A} \sum_{k,l} R^{kl}_i \cdot F^{lk}_j,$$  \hspace{1cm} (2.7)$$
Figure 2.9: (a) A sketch of a particle (center disk) in contact with three other particles (partially shown), where $\vec{R}^{kl}$ is the vector pointing from the center of $k$ to the contact point with $l$ and $\vec{F}^{lk}$ is the force acted on $k$ from $l$. (b) The corresponding eigenvectors of the fabric tensor ($C_1$ and $C_2$) and stress tensor ($\sigma_1$ and $\sigma_2$) from (a), with their lengths indicating the eigenvalues.

where $A$ is the area associated with all the force bearing particles. $\sigma$ is symmetric for a particle or a force network that is in force and torque balanced. In 2D, the normal stress, i.e. pressure $P$, and the shear stress $\tau$ can be determined from $\sigma$ by:

$$P = (\sigma_1 + \sigma_2)/2 \quad \text{and} \quad \tau = |\sigma_1 - \sigma_2|/2,$$

where $\sigma_1$ and $\sigma_2$ are the eigenvalues of $\sigma$. Furthermore, the stress anisotropy can be characterized as $\tau/P$. 
Microscopic Origins of Shear Jamming

Understanding the transition of fluid-like to solid-like granular states, i.e. jamming, is of great theoretical and practical interest [19, 69]. Spherical grains with friction coefficient $\mu$ jam isotropically above a packing fraction, $\phi^\mu_J$ [18, 31]. For frictional grains (discs) [43, 35] with $\phi_S < \phi < \phi_J^0$ there are unjammed, jammed, or highly anisotropic fragile states [35, 36]. According to recently reported data, $\phi_S < \phi_J^\mu$ [31, 35]. Shear jamming (SJ) in a closed system [35] and dilation in a deformable system [37] presumably share a similar origin. SJ has also been reported in suspensions [44, 45, 46], granular impacts [47] and flow [48]. Nevertheless, the origins of mechanically stable force and contact networks associated with SJ for frictional systems remains unclear. The nature of shear jamming in frictionless systems is still under investigation [40, 41, 42, 38, 39]. Since force networks play key roles in shear jamming, understanding their origins is of broad importance. In this chapter, I use physical experiments and analysis to show shear jamming in a frictional granular system and the breakdown of a widely applied theory (shear transformation zones) in sheared systems to explain shear jamming, and propose new microscopic origins for creating stress and mechanical stable force chains during shear, which account for
shear jamming. Then I use experimental data to show the validity of the proposed mechanisms.

Experiments involved shearing a quasi-2D system of photoelastic discs, using the simple-shear apparatus described in Chapter 2 with a base that deformed affinely with the boundaries, providing spatially uniform $\phi$ [43]. The system contained approximately 1000 bi-disperse photoelastic (Vishay PSM-4) discs (friction coefficient $\mu \approx 0.7$) of diameters 16 mm and 12.8 mm in a ratio 1 : 3.3 (large to small) whose optical properties under cross polarization yielded forces on each particle [68]. Data were obtained for five experiments for each of five $\phi$'s in which $0.758 \leq \phi \leq 0.816$. Before each experiment, the inter-particle forces were relaxed to zero by tapping. Shear strain was applied in steps of $\delta \gamma = 0.0027$. After each step, we obtained images yielding positions, rotations and photoelastic responses of all particles after letting the system relax for 6 seconds. These data yielded contact forces, $f$, contact numbers on each particle, $Z$, and the force-moment and stress tensors [68]. Particles are tracked throughout the whole strain steps by using an algorithm developed by Crocker et al. [70].

3.1 Shear Jamming

Representative responses of the system to simple shear at different shear strains are shown in Fig. 3.1 for one run with $\phi = 0.805$. Starting from a stress-free state, the system develops more and more extensive force and contact networks as shear strain $\gamma$ increases, ending up with a rigid percolated force network that is mechanically stable, i.e. a shear jammed state. This specific run will be used to show representative results of the analysis proposed in the following part of this chapter, unless otherwise noted.

A system can be determined to be shear jammed based on $Z$, pressure $P$, or the force network percolation [35]. Here, I choose $Z$ as the criterion, i.e. a system is deemed to be shear jammed if $Z$ averaged over all non-rattler (NR) particles
Figure 3.1: Representative polarized images of a system under simple shear with \( \phi = 0.805 \) at different shear strains: (a) \( \gamma = 0 \), (b) \( \gamma = 0.0594 \), (c) \( \gamma = 0.0918 \), and (d) \( \gamma = 0.1188 \). Starting from a stress-free state (a), particles start to make contacts and form force chains, shown by the photoelastic response, mainly in one diagonal direction, e.g. (b). As more and more force chains form (part (c)), the force network starts to percolate in the other diagonal direction and hence leads the system to the shear jammed regime (part (d)).

\( Z_{\text{iso}} \) is the minimum for mechanical stability in frictional systems under isotropic conditions [19, 69, 35]. Shear jamming is observed for all the densities considered here (0.758 \( \leq \phi \leq 0.816 \)). Starting from an initial state of \( P = 0 \), shearing led to a jammed state with \( Z \geq 3 \), as in the \( Z \) vs. \( f_{NR} \) data of Fig. 3.2(a) (red circles), where \( f_{NR} \) is the fraction of non-rattlers [35]. Here, \( \phi = 0.805 \), and only non-rattlers, are included. \( Z \) grows gradually from \( Z \approx 2.5 \) and at some point exceeds 3. Fig. 3.2(a) also shows the fraction of particles with contact numbers, \( N_{i}/N_{NR} \) vs. \( f_{NR} \) for the same run. \( N_{NR} \) is the total number of non-rattler particles and \( N_{i} \) is the number of particles with \( Z = i \) for \( i \geq 2 \). Initially, the
Figure 3.2: (a) Blue symbols: Fraction of non-rattler particles with the indicated normalized number of contacts. Red circles: The coordination number, $Z$, vs. the fraction of non-rattlers, $f_{NR}$, for one run with $\phi = 0.805$. (b) Data for $N_i$, the total number of particles with a given number of strong ($f \geq \bar{f}$) contacts (and possibly other weak contacts), normalized by $N$, the total number of particles in the system. The color bar gives the average $Z$, including weak contacts, for a given symbol. (c) Similar data as in (b), for particles with at least one moderate ($0.5 \bar{f} < f < \bar{f}$) force excluding strong forces.
majority of non-rattlers have $Z = 2$, but $N_2/N_{NR}$ decreases with $\gamma$ or $f_{NR}$, and the fraction of non-rattlers with $Z = 3$ and eventually $Z = 4$ become more important. The data for $i \geq 3$ provide a reasonable measure of branches.

The relation between a particle’s contact number and the mean force it experiences is also relevant. Hence, particles with one or more contact forces, $f$, in a given range, should be taken into consideration. ‘Strong force particles’ have one or more $f \geq \bar{f}$, where $\bar{f}$ is the system-mean force at a given $\gamma$. Particles with one or more $f$’s in $0.5\bar{f} < f < \bar{f}$ belong to the ‘moderate’ network; those with $f < 0.5\bar{f}$ are in the weak network, or are rattlers. Such a choice of thresholds has been proven to be valid through a k-core percolation analysis by Bi et al. [35].

Fig. 3.2(b) shows data for $N_i$, the total number of particles with $i$ strong contacts (and possibly other weaker contacts), normalized by $N$, the total number of particles in the system. Here, the color gives the mean $Z$ for particles represented by each symbol. For instance, the crosses give the number fraction of particles with exactly two strong contacts, with possibly other contacts. Initially, these particles have $Z$ close to 2, but as $f_{NR}$ increases, $Z$ reaches $Z \sim 3$ near $f_{NR} \simeq 0.7$. Particles with exactly two strong contacts are force-chain-like particles, and clearly these dominate the strong network. In terms of the force network, initially, quasi-linear force chains (with strong binary contacts) dominate the strong network. But, as shear progresses the force chain particles gain contacts, modifying the force chains structure as force chains emerge in the dilation direction. This is a hallmark of shear jamming.

As the system moves toward shear jamming, particles with two strong contacts still dominate, e.g. Fig. 3.2(b), but such particles gradually add more contacts, often initially weaker, with continued shear. However, particles with moderate forces are also of interest. We consider particles that have one or more contact forces in $0.5\bar{f} < f < \bar{f}$, and no contact forces above $\bar{f}$. Fig. 3.2(c) shows data for the fraction of particles that have moderate force contacts vs. $f_{NR}$. As shear is applied, the
Figure 3.3: (a) Particles displacements, (b) non-affine displacements, and (c) a blow up of a region for the non-affine displacements in (b), following a simple shear strain of $\gamma = 0.0999$, when the system just reaches a shear jammed state, in units of the small particle radius $R$. The blue arrows in (b) and (c) are amplified by 3.5 times the actual displacement. The non-affine particle displacements are the actual particle displacement minus the displacement that the particle would have if it exactly followed the applied strain. The simple shear direction is along $y$ axis, as indicated by the red arrows.
number of moderate force particles tends to grow. This is particularly apparent for the two-contact moderate force particles, which significantly increase in number upon approaching shear jamming, then decrease as the number of strong force particles grows, e.g. Fig. 3.2(b).

Next particle motion during shear is considered. Particle displacements tend to closely follow the affine strain, as shown in Fig. 3.3, which gives both the total (Fig. 3.3(a)) and the non-affine motion (Fig. 3.3(b)), i.e. the actual motion of particles minus the local affine displacements, of individual particles. Thus, shear jamming occurs due to very small relative motion of grains, which happens mainly due to particle collisions with their nearby neighbors.

3.2 Microscopic Origins: Trimers and Branches

In order to explain the emergence of mechanically stable force and contact networks during linear shear, a mechanism is needed to connect particle displacements to the increase in $Z$, both of which are induced by shear. Essentially, shear consists of compression in one direction and dilation in the other, e.g. Fig. 3.4(a-b). Utilizing such a combination of compression and dilation, shear transformation zones (STZ’s), a much studied model in deformation and failure of sheared particulate systems [52, 57, 58, 59]. A T1 event is a minimal STZ, e.g. Fig. 3.5(a-b), and corresponds to pure shear at the particle scale. STZ’s have also been applied to granular systems [54, 71, 72]. During failure of a frictional granular system, Tordesillas et al. [73] show that buckling of existing force chains is the key mesoscopic failure mechanism in this case.

However, both STZ’s and force chain buckling are failure mechanisms, which is opposite to building up stress and force chains during shear, which accounts for the principal process during shear jamming. In addition, the force networks that are key
Figure 3.4: (a) Sketch of simple shear with solid lines showing the principal strain directions, and neutral lines (dashed) along which there is neither compression nor dilation. (b) Sketch of pure shear showing principal directions and neutral lines similar to those of (a). In (a) and (b), the shaded regions undergo compression.

to shear jamming observed in experiments, e.g. Fig. 3.1, are quasi-linear segments and lack neighboring chain segments. As a force chain deforms, the constituent particles do not show T1-like events, e.g. configurations from Fig. 3.5(a) to Fig. 3.5(b), because that would require two adjacent chains, which are highly improbable, due to the frictional nature of contacts. Therefore, STZ’s, though applied successfully to a lot of amorphous systems, do not fit here for explaining the microscopic origin that enables shear jamming in frictional granular systems.

In the remainder of this chapter, I propose new and different mechanisms that account for shear jamming based on experimental observation and analysis: trimers (Fig. 3.6), which are linear sequences of three particles with the center particle in contact with the other two, and branches, which occur at the convergence of three or more force chains. I will explain the model of trimers and branches, identify all trimers/branches and show: 1) that trimers that are roughly straight and in the compression direction, and 2) that branches involving intersections of force chain segments, play central roles in the shear jamming process.

Force chains, which carry the majority of the forces, are roughly straight line segments, typically containing a modest number of particles, as in Fig. 3.1. To characterize the evolution of chains, two things are needed: 1) a basic building block
Figure 3.5: (a-b) Sketch of a T1 event for a group of four frictionless grains under pure shear. (c) Hypothetical lines of mechanically stable frictional particles, e.g. 5-1-2-3-6, only exist if the centers are located along the two dashed lines as sketched. Such a configuration has a tiny probability of occurrence for more than a few grain lengths, and is unstable to small system changes, such as shear as sketched in the figure.

that accounts for their local bending/curvature, and 2) an accounting of branches. A minimal structure for 1) is captured by considering three consecutive particles in a chain, which I call a trimer. Branches occur where three or more force chain segments converge. Their existence reflects the random structure of packings, and the improbability of finding long stable chains with only two contacts per particle, e.g. Fig. 3.5(c). However, three or more force chain segments terminating at a common particle can form a stable structure.

In general, a trimer, Fig. 3.6, is any three particles (e.g. 1, 2, 3), such that the central particle contacts the other two. There are many trimers, or potential trimers, where a central particle (almost) touches two neighbors, but only a modest fraction of trimers in a force free state become part of force chains at shear jamming. Key
Figure 3.6: A sequence of three frictional grains (solid circles with numbers indicating indices) forms a trimer. The relevant geometric properties of a trimer include a measure of how straight it is, and its orientation relative to the principal strain directions of applied shear. Here, the straightness of the trimer is characterized by $\theta$, and the orientation is characterized by $\alpha$, the angle between the principal strain axis, and the line through the contacts between particles 1 and 2 and between particles 2 and 3. C and D indicate the directions of compression and dilation, respectively. \( \hat{b}_i \) (not shown) is a unit vector from the center of grain 2 to the contact with grain \( i = 1, 3 \). Numbers indicate the indices of the corresponding grains.

Geometric properties that determine which trimers might form force chains include how straight they are and whether they are roughly aligned with the compressive shear direction. That is, force chains tend to form as particles in roughly straight trimers are pushed together in the compressive direction.

For a trimer, e.g. Fig. 3.6, that is bent at an angle $\theta$, the central particle can be mechanically stable with only two contacts providing $\theta < \theta_\mu$, where $\tan(\theta_\mu) = \mu$, and $\mu$ is the inter-particle friction coefficient. But, a series of trimers forming a chain can only be stable in the absence of other contacts if they are aligned as shown in
Fig. 3.5(c), which is highly improbably for chains with more than a few particles. And such a chain is unstable to small applied stress/strain. One way to understand this instability is to note that isolated central particles in trimers have \( Z = 2 \), which is below \( Z_{\text{iso}} \) for 2D frictional packings.

Roughly straight trimers respond differently depending on the angle \( \alpha \) between the compression direction and the contact direction, i.e. the line passing through the two contacts experienced by particle 2. Particles in a trimer with small \( \alpha \), i.e. aligned towards the compression direction, experience compression that pushes particles 1 and 3 together, tending to bend the trimer and increase \( \theta \). By contrast, particles in large \( \alpha \) trimers (i.e. in the dilation cone) tend to exhibit nonaffine motion induced by neighboring particles responding to compression. The present experiments provide a weak frictional force from the deforming base, but that is easily overcome by collisions from other particles. Shear also tends to rotate trimer orientations.

Of particular interest, shear strain leads to compression and hence bending of trimers that are roughly aligned with the compression direction. Consider a simple example where \( \alpha = 0 \), the trimer is aligned with the compression direction, and \( \theta \) is not large. Referring to Fig. 3.6(c), the action of pushing particle 1 towards particle 3 (e.g. along the y-direction) pushes particle 2 in the negative x-direction faster than the affine dilation. Suppose that trimer particles 1 and 3 are located at \((x, y) = 2R(0, \pm \cos \theta) \) (\( R \) is the particle radius) and that particle 2 is at \((x, y) = -2R(\sin \theta, 0) \). Compressively bending the trimer, keeping 1 and 3 on the y-axis and 2 on the x-axis (e.g. increasing \( \theta \)) displaces 2 by \( \delta x_\theta \) and 1 and 3 towards the origin by \( \delta y_\theta \), where \( \delta x_\theta / \delta y_\theta = \cot \theta \). This trimer is part of a system that undergoes pure shear with compression along y, e.g. \( y_o \to y_o/(1 + \gamma) \) and dilation along x, e.g. \( x_o \to x_o(1 + \gamma) \) (\( \gamma \) assumed small). The affine shear maps the centers of 1 and 3 to \((x', y') = (0, \pm 2R \cos \theta/(1 + \gamma)) \), which corresponds to a displacement of these points by \( \delta y_{\text{aff}} = -2R \gamma (1 + \gamma)^{-1} \cos \theta \). The affine strain maps the center of
particle 2 to \((x', y') = (-2R(1 + \gamma) \sin \theta, 0)\), which corresponds to a shift \(\delta x_{aff} = -2R\gamma \sin \theta\). If the trimer responds to the applied shear such that particles 1 and 3 move towards each other along the y direction by \(\delta y_{aff}\), which is likely because the boundaries are pushing particles together in this direction, particle 2 will be pushed to the left by a different amount than the affine strain \(\delta x_{aff}\). Because the dilation direction boundaries are moving outward in the dilation direction, there is little initial resistance to the leftward motion of 2. The ratio \(\delta x_{\theta}/\delta x_{aff} = \cot^2 \theta (1 + \gamma)^{-1}\), which for \(\gamma = 0.2\), is greater than unity for \(\theta < 0.236\pi \simeq \pi/4\). Even for rather large \(\theta\), the compressive motion pushing 1 and 3 together pushes 2 to the left faster than the dilation. For monodisperse particles, \(\theta \leq \pi/3\), so for trimers aligned along the compression direction, pushing the outer particles together is highly effective at pushing the central particle in the dilation direction.

The above process leads naturally to the generation of an additional contact, e.g. between particles 2 and 4 in the sketch of Fig. 3.6, bringing the contact number for particle 2 to 3. In general, the forces acting on 2 from 1 and 3 tend to be stronger (weaker) in the y (x)-direction, hence, the forces between 2 and 4 generated by bending are initially weak. This is effectively a kind of mechanical advantage, where motion to the left by 2 is amplified relative to that of 1 and 3, but where the resulting force between 2 and 4 is likely be smaller than those between 1 and 2 and between 3 and 2. Crucially, this provides a mechanism for raising \(Z\) to values that approach the isostatic value, i.e. 3, to create a weak network in the dilation direction, and to generate local dilation.

It is expected that such a trimer bending effect still applies if the alignment is not perfect, which enhances the weak force network. Importantly, this mechanism can lead to the formation of branches (where the central particle has \(Z \geq 3\)), shear jamming and ultimately dilatancy, with only moderate relative motion of particles. In addition, trimer bending corresponds to local displacements that break symmetry,
e.g. particles 1 and 3 move symmetrically about the x-axis, but there is no mirror image particle for 2 in general. Both branches and the bending of trimers, which can create branches, provide ways to establish stable force networks.

3.3 Results and Discussion

With the mechanisms proposed above, I come back to the experimental data shown earlier in Section 3.1 to test this model. First, representative trimers are studied extensively to verify the response of trimers with different $\alpha$. An example region is shown in Fig. 3.7, where particles are indicated by numbers, i.e. their identities given by the tracking algorithm. In the red boxes of Fig. 3.7, particles 723-744-753 form a trimer in the compression cone. In the white boxes, particles 679-687-708 form a trimer in the dilation cone, and particles that become branches as $\gamma$ increases, e.g. particles 689 and 690 in Fig. 3.7(d). Then, a geometric measure accounting both $\theta$ and $\alpha$ is defined to characterize trimers collectively.

3.3.1 Trimer in the Compression Cone

Fig. 3.8 tracks the geometric and force response of a particular trimer, particles 1, 2 and 3, with typical features for trimers in the compressive cone. Fig. 3.8(a)-insets show photoelastic images of the region around the trimer. At first, Fig. 3.8(b), the trimer bends slowly with $\gamma$, i.e. $|\theta|$ increases, and rotates somewhat faster than the affine strain, e.g. $\alpha$ increases slowly. The bending process is not locally symmetric: no mirror-image trimer bends (here and generally) in the opposite direction. Initially, there is no force on particle, 2, but at $\gamma \approx 0.051$, the pressure $P$ on particle 2 shows a sharp transition, and $P$ grows roughly linearly with $\gamma$ (Fig. 3.8(a)). At this point, particle 2 has no other force bearing contacts, and the growth in $P$ is only due to the compressive strain from 1 and 3 pushing against 2 in Fig. 3.6. At $\gamma = 0.0918$, $\theta$ shows a sharp transition, and the trimer bends much more rapidly with $\gamma$. This bending
Figure 3.7: Blowups of part of the system at several strains: (a) $\gamma = 0$, (b) $\gamma = 0.0594$, (c) $\gamma = 0.0918$, and (d) $\gamma = 0.1188$. The yellow numbers are the tracking indices for each particle and the green circles indicate the edges of particles. The red box in each subplot encloses particles 723, 744 and 753, which form a trimer bending in the compression direction as discussed in the main text. The white boxes indicate a region where a branch emerges by $\gamma = 0.0918$ (part c). Other branches form by $\gamma = 0.118$ (part d). The white boxes also enclose particles 679, 687 and 708, which form a trimer in the dilation direction. Fig. 3.10 provides quantitative information on this trimer. Shear directions are indicated by the cyan arrows.
Figure 3.8: Representative example of trimer response to shear strain $\gamma$. (a) $P$ for particle 2 (circles) and photoelastic images of the trimer (particles 1-2-3) at various stages. Contact number for particle 2 is indicated by different symbols. When $\gamma = 0.1161$, particle 2 contacts particle 4, and $P$ on 2 starts to rise quickly. When $Z = 4$, particle 2 makes a very weak contact with particle 5, which is barely visible in the inset image. The lab frame is indicated in the inset as the Cartesian coordination system $x$-$y$, and shear is along the $y$ axis. The compression direction is roughly along $45^\circ$. (b) shows the opening angle, $\theta$ (black triangles), and orientation $\alpha$ (red circles) of the trimer.
Figure 3.9: Representative example of trimer (particles 1-2-3 in the insets of Fig. 3.8(a)) dilation for the center particle. (a) Blue circles: The distance from the center particle of a trimer to the line connecting the centers of the other two particles. Red open squares: Also plotted as a comparison is what the distance would be if every particle moved affinely with the applied shear strain. The green dashed line indicates when the center particle first contacts the other two particles, and the black dashed line indicates when the center particle makes an extra contact with particle 4. The inset shows the ratio of these two distances (blue/red). (b) The pressure of the center particle, $P$, vs. its volumetric strain $\epsilon^V$, during the same strain interval in (a). No obvious correlation is found between $P$ and $\epsilon^V$.

creates a force-bearing contact between 2 and 4 when $\gamma = 0.1161$, hence a branch. This initially weak contact is along the dilation direction, and is associated with a second transition in the $P$ vs. $\gamma$ data for 2. Eventually, more complex behavior occurs; $P$ on particle 2, $\alpha$, and $\theta$ all grow. By the end, $\theta \approx 30^\circ$, which is nearly double its initial value. The force network in the dilation direction associated with 4 has grown significantly.

For the above trimer example, it can be shown that the bending process pushes the central particle (2) towards the neighbor (4) faster than the affine dilation. Fig. 3.9(a) plots the distance from the center of particle 2 to the line connecting the centers of particles 1 and 3 (blue circles). Also plotted (red squares) is the same distance that would be traveled if all the particles had only affine displacements. Clearly the actual distance increases faster than that the affine shear strain. The inset plots the ratio of
these two distances (blue/red), which is greater than 1 during the process of trimer bending.

In addition, the cross-coupling between pressure and the local volumetric strain ($\epsilon^V$) associated with particle 2 is investigated in Fig. 3.9(b). Here $\epsilon^V$ is computed from a strain field, which is a best fit result by taking particles displacements of the nearest neighbors of particle 2 into consideration. The region around particle 2 shows local shear dilatancy ($\epsilon^V > 0$), although it is not tightly coupled to the local pressure change. By contrast, other studies show that these two quantities are well correlated (linear relationship with a negative slope) while investigated globally in a system of frictionless particles undergoing either isotropic or uniaxial compression [74]. Such a discrepancy of the behavior of $P$ vs. $\epsilon^V$ in the shear induced dilation from that in the compression case indicates a clear difference in the modes of shear and compression, as well as in systems with and without friction.

3.3.2 Trimer in the Dilation Cone

Trimers in the dilation direction usually straighten under shear. Fig. 3.10 shows an example of such a process for the trimer consisting of particles 1, 2, and 3 in Fig. 3.10. These particles lie in the region marked with white boxes in Fig. 3.7, where 1 ↔ 679, 2 ↔ 687 and 3 ↔ 708. Fig. 3.10(b) shows that the opening angle $\theta$ of this trimer decreases by roughly 15$^\circ$ after a total shear strain of 0.18, indicating a significant straightening.

3.3.3 Collective Behavior of Trimers

The above examples typifies trimer bending, creation of new contacts, and the emergence of the network and trimer straightening in the dilation direction. To globally characterize trimer evolution, I define a measure, $O$, that captures the key geometric trimer properties $\theta$ and $\alpha$. Trimers oriented in the compression cone, $|\alpha| < \pi/4$, with
Figure 3.10: Representative example of trimer response to shear strain $\gamma$. (a) $P$ for particle 2 (circles) and photoelastic images of the trimer (particles 1-2-3) at various stages. Contact number for particle 2 is indicated by different symbols. When $\gamma = 0.1161$, particle 2 contacts particle 4, and $P$ on 2 starts to rise quickly. When $Z = 4$, particle 2 makes a very weak contact with particle 5, which is barely visible in the inset image. The lab frame is indicated in the inset as the Cartesian coordination system x-y, and shear is along the y axis. The compression direction is roughly along $45^\circ$. (b) shows the opening angle, $\theta$ (black triangles), and orientation $\alpha$ (red circles) of the trimer.
moderate \( \theta \) (roughly straight), can become part of a strong force chain during SJ. Trimers in the dilation cone, |\( \alpha > \pi/4 \)|, evolve during SJ, but are not particularly important for creating new contacts or enhancing the force networks for \( \gamma < \gamma_{SJ} \), the strain needed to reach SJ. A simple though not unique measure with both important geometric properties of a trimer is

\[
O = -[(\hat{b}_i \cdot \hat{b}_j - c_{ij})/\{A(1 + c_{ij})\} \cdot \cos(2\alpha)]
\]

where \( \hat{b}_i \) and \( \hat{b}_j \) are unit vectors from the origin of the central particle (e.g. 2 in Fig. 3.6) to the two other trimer particles (e.g. 1 and 3), and \( c_{ij} \) is the maximum value of \( \hat{b}_i \cdot \hat{b}_j \) (when 1 and 3 touch). \(-[(\hat{b}_i \cdot \hat{b}_j - c_{ij})/(1 + c_{ij})]\) is 1 for a straight trimer and 0 for a maximally bent trimer. \( O \) is positive and bigger for smaller \( \theta \) and \( \alpha \approx 0 \). It is negative and smaller (more negative) for smaller \( \theta \) and orientations closer to the dilation direction. \( O \) will decrease if a trimer in the compression direction bends or if one in the dilation direction straightens. If the normalization constant \( A = 1 \), \( O \) lies in \(-1 \leq O \leq 1 \). Also if \( \theta \) and \( \alpha \) for a collection of trimers are uniformly distributed, the mean value of \( O \) for the compression (dilation) cone would be 0.378 (-0.378) for \( A = 1 \). Henceforth, \( A \) is chosen to be 0.378, so that a uniform distribution of trimers in the compression cone is unit normalized.

The average of \( O \), \( \bar{O} \) is used to characterize the collective properties of a special set (SS) of trimers that form the force network in an experiment at the onset of SJ, e.g. where \( Z \) reaches 3. This provides a collective measure of the response of the most important trimers that might otherwise appear as random motion. Fig. 3.11(a) shows \( \bar{O} \) vs. \( \gamma \) for five runs at \( \phi = 0.805 \), for which SJ occurs at \( \gamma_{SJ} \approx 0.1 \). \( \bar{O} \) starts at a positive value because trimers in the SS, i.e. in the strong network at jamming, are often roughly straight trimers aligned in the compression region. \( \bar{O} \) decreases nearly linearly with \( \gamma \), supporting the expectation that, statistically, force chains in the compression cone bend under shear. \( \bar{O} \) at \( \gamma = 0 \) varies from run to run due to different initial conditions, but the slope \( d\bar{O}/d\gamma \) is nearly the same for each run.
Figure 3.11: (a) \( \bar{O} \), for trimers in the force network at shear jamming for five runs with \( \phi = 0.805 \) – colors and symbols indicate different runs. The black crosses indicate when \( Z \) just reaches 3. (b) Two dimensional PDF of \( O \) vs. \( -\left( \hat{b}_i \cdot \hat{b}_j - c_{ij} \right) / (1 + c_{ij}) \), which characterizes the straightness of a trimer, and \( \cos(2\alpha) \), which gives its orientation with respect to the compression direction. These data are for \( \phi = 0.805 \) run 1 at the step where the system just reaches the shear jammed state in (a). (c) The slope of the curve \( \bar{O} \) vs \( \gamma \), averaged over five runs for each density. (d) \( O \) values averaged over five runs for each density at a certain strain, where blue squares correspond to \( \gamma = 0 \), and red squares correspond to \( \gamma = \gamma_{SJ} \).

As argued in Section 3.2, the response of a trimer to shear depends on its orientation relative to the principal strain directions and on the amount by which it is bent. For instance, relatively straight trimers aligned in the compression direction tend to respond by increasing the pressure on the central particle of the trimer and by bending into the dilation direction. Both effects are important along the road to shear jamming, and \( O \) provides a convenient tool for detecting particles that have...
these properties (or conversely properties that mitigate against shear jamming). The statistics of $O$ for all or part of the system are particularly useful for identifying particular behavior, such as trimers that participate in the force network. $O$ contains one factor that is larger for small $\theta$, i.e. trimers that are relatively straight, and another that is larger when the trimer is oriented more in the compression direction, i.e. in the compression cone. Though conveniently combining these two important geometric properties in one measure, it is still useful to know what role is played by each factor in $O$. Fig. 3.11(b) shows the two dimensional probability function (PDF) for the components of $O$ over the whole force network when the system just reaches the shear jammed state. This PDF is shown as a function of the independent factors $-(\hat{b}_i \cdot \hat{b}_j - c_{ij})/(1 + c_{ij})$ (the $x$ axis), and $\cos(2\alpha)$, the $y$-axis. There are two peaks in the PDF: the largest by far is near $x \sim 1$, $y \sim 1$ and a smaller one is near $x \sim 0$ and $y \sim -1$. Thus, there are two significant features: the smaller corresponds to largely bent trimers in the dilation direction and the second corresponds to fairly straight trimers in the compression direction. It is the latter that corresponds to much of the strong force network.

The behavior of $O$ may be affected by varying $\phi$. To investigate that, the slope, $d\bar{O}/d\gamma$, averaged over five runs for each density, is first plotted against $\phi$ in Fig. 3.11(c). There seems to be a weak non-monotonic trend of the slope as $\phi$ increases. However, such a trend is not clear within the error bars. Nevertheless, the decay speed, the negative of $d\bar{O}/d\gamma$, at both the lowest $\phi$ and the highest $\phi$ is smaller than that at $\phi = 0.805$. Different mechanisms may contribute to such a behavior: at lower $\phi$, particles are sparsely distributed in the system, which decreases the probability that particles make contacts, and hence reduces the possible trimer bending; at higher $\phi$, the probability of making contacts with neighbors before a trimer bends too much is fairly high, which also slows down trimer bending. Both reasons can contribute to a smaller decay speed.
Then, more interestingly, Fig. 3.11(d) compares $\bar{O}$ at $\gamma = 0$, and at SJ. Given that the data in Fig. 3.11(a) only correspond to the fraction of trimers that become part of the strong network at jamming, the initial values of $\bar{O}$ are significant. $\bar{O}(\gamma_{SJ}) > 0$ is less than $\bar{O}(0)$, and is nearly independent of $\phi$, indicating a common/universal $\bar{O}$ at SJ. The nonzero value of $\bar{O}(\gamma_{SJ})$ indicates an anisotropic network when the system reaches a shear jammed state. The fact that $\bar{O}(0)$ increases as $\phi$ decreases towards $\phi_{S}$, the lower limit for SJ, indicates that the force network at jamming draws increasingly from trimers that tend to be straighter and more compression-aligned.

Furthermore, I look into the relation between the geometric properties of trimers and their role in shear jamming by computing $P_{r}$, the pressure for trimers, rescaled by $P$ at jamming, above and below the threshold, $O = 0$, as shown in Fig. 3.12. The data points in Fig. 3.12(a) show $P_{r}$ for particles belonging to all trimers with $O \geq 0$. Remarkably, all the data from different densities tend to collapse at and above $\phi_{SJ}$, indicating universal behavior when expressed as functions of $f_{NR}$. The contribution from the remainder of the particles is indicated by the dashed lines, which is a fit for $P_{r}$ in (b).
for $P_r$ vs $f_{NR}$ in Fig. 3.12(b). Clearly $P_r$ for $O \geq 0$ dominates and begins to rise at a significantly lower $f_{NR}$ than $P_r$ for the $O < 0$ trimers. Thus, $O \geq 0$ trimer particles form the backbone of force networks in the shear jammed state. As for the particles that belong to trimers below the threshold, $O = 0$, $P_r$ shows a sharp transition at $f_{NR} = 0.8$, which is close to the shear jamming point, for different packing fractions $\phi$. This sharp transition again validates the use of $O$ as a filter: trimers with $O$ below the threshold contribute little to the pressure until very close to shear jamming transition, when the force networks start to percolate throughout the system.

3.4 Conclusions

In summary, I have proposed novel structures and mechanisms enabling shear jamming for frictional discs: 1) particular trimers, roughly straight triplets of particles aligned in the compression direction, strengthen and bend under shear, pushing particles in the dilation direction faster than the affine dilation; and 2) branches, which connect force chain segments. Trimer bending helps generate the weak transverse network, increases $Z$ and the number of branches. Trimers with moderate $\alpha$ typically show compression–increasing local pressure, bending, and rotation. The filter $O$ identifies collective geometric trimer properties, and is correlated with the particles carrying the majority of the forces/pressure. Branches provide a second mechanism for generating stable structures and for raising $Z$ above $Z_{iso}$. The fraction of particles with strong ($f \geq \bar{f}$) or moderate contact forces ($0.5 \bar{f} < f < \bar{f}$) also provides key insights into the roles of 2- and 3-contact particles vs. those with more contacts.

Trimer bending and branch formation are not unique to shear. They presumably occur during compression in one or more directions. Since the resulting force networks, particularly for shear jamming, are anisotropic, bulk response functions must reflect this anisotropy. Force networks and microscopic structures in three dimen-
sions present a future challenge, where generalized trimer bending may be relevant. The mechanism of trimer bending considered here for frictional particles may well apply for frictionless particles. For the former case, enough bending must occur to reach a $Z$ of a bit more than 3. In the frictionless case, if bending occurs, larger bending angles may be needed to reach the 2D $Z_{iso} = 4$ for frictionless particles. It would be very interesting to see if this effect does indeed occur in the frictionless case of simulations or possibly very low friction experiments.
In the previous chapter, I have proposed a new and different mechanism other than shear transformation zones, i.e. trimers and branches, to explain the microscopic origins of shear jamming. In that model, trimers, particularly, require the existence of friction for mechanical stability. Otherwise, there can only be straight stable isolated trimers, namely $\theta = 0$, for frictionless particles. Clearly friction plays an important role in SJ. Since originally reported in a frictional granular system \cite{35}, shear jamming has stimulated many studies of frictionless systems, mainly using numerical simulations. The nature of shear jamming in frictionless systems is still under investigation \cite{40, 41, 42, 38, 39}. The concept of shear jamming has also been utilized to explain discontinuous shear thickening in non-Newtonian suspensions, where the discontinuity in shear viscosity as the shear rate varies is believed to be caused by granularlike frictional contacts between suspended particles at high shear rate \cite{44}. In order to understand the effect of friction on shear jamming in this chapter, I study granular systems with various inter-particle friction coefficients, $\mu$.

Experiments involve applying quasi-static linear simple shear to granular systems consisting of bi-disperse photoelastic discs with different inter-particle $\mu$. Standard
Figure 4.1: Representative examples of particles with different friction coefficients $\mu$. (a) - (d): particles wrapped with Teflon tape, resulting in $\mu = 0.15$. (e) - (h): standard particles with $\mu = 0.7$. (i) - (l): particles cut with fine teeth on their edges, providing an extremely large friction coefficient. At each row, from left to right: a closeup of particles edges, an example ‘N’ image, an example ‘P’ image, and an example ‘U’ image. In (k), two particles are highlighted by red dashed circles, which indicate the friction coefficient must be at least $\sqrt{3}$.

particles (discussed in Chapter 3) have $\mu = 0.7$, which are also the ones used in the experiments described in Chapter 3. Then a layer of Teflon tape is wrapped around the side to reduce $\mu$ to 0.15. In order to have a higher $\mu$, another kind of particles is made with fine teeth on the edge, so that particles cannot slide against each other when they become interlocked. Examples of all three kinds of particles are shown in Fig. 4.1. From this point till the end of this chapter, I will refer to particles with $\mu = 0.15$, $\mu = 0.7$, and fine teeth as $\mu_l$, $\mu_m$, and $\mu_h$ particles, respectively. A more
Table 4.1: Dimensions for three kinds of particles with different inter-particle friction coefficient.

<table>
<thead>
<tr>
<th>Particle Friction</th>
<th>Diameter Big (mm)</th>
<th>Diameter Small (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu = 0.15 = \mu_L$</td>
<td>16.55</td>
<td>13.36</td>
</tr>
<tr>
<td>$\mu = 0.7 = \mu_m$</td>
<td>16</td>
<td>12.8</td>
</tr>
<tr>
<td>$\mu = \mu_h$</td>
<td>15.91</td>
<td>13.05</td>
</tr>
</tbody>
</table>

detailed description for the dimensions of these three kinds of particles can be found in Table 4.1.

A typical linear shear experiment consists of repeating the following procedure until a certain strain $\gamma$ is achieved: applying a small shear step ($\delta \gamma = 0.0027$) to an initially stress-free system at a certain $\phi$, followed by letting the system relax for a few seconds and then taking three kinds of pictures to record particle positions, orientation and inter-particle forces. $\phi$ can be changed by increasing or reducing the number of particles in the system, while maintaining the number ratio the same, i.e. 1 : 3.3 (large to small). In general, the number of particles in the system is of the order of 1000. Different $\phi$’s are tested with each $\phi$ repeated five times with different initial configurations, whose span depends on $\mu$. For a higher $\mu$, particles tend to pop out of plane more easily at high $\phi$ due to strongly anisotropic force networks and extremely large contact forces, limiting the highest $\phi$ that can be tested. All the $\phi$’s lie below the isotropic jamming point for the frictionless system, $\phi_J = 0.84$ [18].

4.1 Shear Jamming for Different $\mu$

Shear jamming is observed for all three $\mu$’s. Representative examples of the photomechanical response of systems of different $\mu$’s at the same $\phi = 0.805$ are shown in Fig. 4.2.

Referring to the shear jamming phase diagram shown in Fig. 1.4, points of interest are $\phi_J$, the isotropic jamming point, and $\phi_S$, the lowest packing fraction for the
Figure 4.2: Representative examples of systems under shear with different friction coefficients $\mu$. (a) - (c): $\mu = 0.15$; (d) - (f): $\mu = 0.7$; (g) - (i): particles with fine teeth on their edges. At each row, panels from left to right show the system states as shear strain increases: from a stress free state (left), to a fragile state where most force networks are oriented close to the compression direction of shear (middle), and to a shear jammed states where the force networks percolate throughout the system and form a rigid material (right).

system below where shear jamming can never happen. Also of importance are the transitions from the fluid-like state to the fragile state (mechanically stable to forward shear, but unstable shear direction reversal), and from fragile to shear jammed state. In that phase diagram, the two control parameters over the state of the system are shear stress $\tau$ and packing fraction $\phi$. However, during experiments, due to the design and limitation of the setup, only $\phi$ and the shear strain $\gamma$ are well controlled. Therefore, instead of looking at $\tau$, first the shear strains at particular transitions, e.g. transitions from fluid-like to fragile states and from fragile to shear jammed states, are investigated.
Determining the state of a system is based on force network percolation: a system is deemed to be in a fragile state if the force network connects two boundaries of the shear box but not all four, and in a shear jammed state if the force network connects all four boundaries. Such criteria have been validated by Bi et al. [35]. By these criteria, the onset shear strains at which transitions from fluid-like to fragile states and from fragile to shear jammed states happen, denoted as $\gamma_F$ and $\gamma_{SJ}$, respectively, are shown in Fig. 4.3.

The behavior of either $\gamma_F$ (Fig. 4.3(a)) or $\gamma_{SJ}$ (Fig. 4.3(b)) vs. $\phi$ for different $\mu$ are quite similar. So here I will focus on just one onset shear strain, e.g. $\gamma_{SJ}$. For any $\mu$, as $\phi$ increases towards the isotropic jamming point, the strain needed for a system to become shear jammed from a stress-free state decreases monotonically. This can be easily understood by the higher packing fraction allowing more frequent particle contacts during strain. Besides, for a fixed $\phi$, $\gamma_{SJ}$ increases as $\mu$ decreases. This observation indicates that it is more difficult to shear jam a system as lowering $\mu$. Due to the limitation of current experiment techniques, no particles showing photoelastic properties with fairly low $\mu = \mu_l$ or even $\mu = 0$ are accessible. Such a limitation remains as a future challenge to overcome to investigate the frictionless
Figure 4.4: The same data from Fig. 4.3, plotted vs. a rescaled packing fraction \((\phi_C - \phi)/(\phi - \phi_S)\), where \(\phi_C\) is chosen to be the isotropic jamming point, 0.84 and \(\phi_S\) is the lowest \(\phi\) for shear jamming to happen. \(\phi_S\) equals 0.78, 0.74, and 0.69 for \(\mu = \mu_l, \mu_m\) and \(\mu_h\), respectively.

In order to understand the difference/similarity of different \(\mu\) systems, a rescaling of the packing fraction \(\phi\) is applied. \(\phi\) is rescaled as \((\phi_C - \phi)/(\phi - \phi_S)\), where \(\phi_S\) and \(\phi_C\) serve as the lowest and highest packing fraction at which a system can be shear jammed, respectively, and given by the best fit. Surprisingly, all the data for \(\gamma_F\) and \(\gamma_{SJ}\) collapse into a single curve when plotted against the rescaled packing fraction, as shown in Fig. 4.4. Such a collapse indicates that although quantitatively different, the fragile/shear jamming transition for systems with different \(\mu\)’s is presumably universal, when \(\mu > 0\). In Fig. 4.4, \(\phi_C\) is chosen to be 0.84, which is the isotropic jamming point for the frictionless discs. And the best fit reveals \(\phi_S\) to be 0.78, 0.74 and 0.69 for \(\mu\) from low to high, respectively. Hence, by increasing \(\mu\), the lower end of \(\phi\) below which shear jamming cannot happen decreases. In comparison, these values are lower than the corresponding isotropic jamming point obtained from frictional simulations by Silbert [31]. Moreover, the fact that \(\phi_S = 0.69\) for the largest \(\mu\) tested is less than the random loose packing validates the existence of shear jamming in nature and indicates a possibly intrinsic difference between shear jamming and
isotropic jamming.

4.2 Pressure Response

In addition to the onsets of $\gamma$ for fragile and shear jammed states, the mechanical response under shear also shows a clear difference, e.g. Fig. 4.2. In particular, the behavior of the pressure $P$ depends on $\mu$, as shown in Fig. 4.5(a). $P$ increases faster with $\gamma$ for a system with higher $\mu$, at a fixed $\phi$. It has been shown by Ren et al. for $\mu = 0.7$ that $P$ goes up approximately quadratically with $\gamma$ [43]. This quadratic relationship is shown in Fig. 4.5(b) where $P$ increases roughly linearly when plotted vs. $\gamma^2$. A simple yet effective measure of how fast $P$ increases with $\gamma$ can be defined as $(\partial^2 P/\partial \gamma^2)/2$. Since shear jamming in a closed system and dilation in a deformable system, i.e. Reynolds dilatancy [37], presumably share a similar origin, such a measure of the speed is denoted as the Reynolds coefficient, or $R$ here.

Results for $R$ with different $\phi$ and $\mu$ are shown in Fig. 4.6. As $\phi$ approaches the isotropic jamming point from below, $R$ increases dramatically in all the three cases with different $\mu$. Moreover, for a certain $\phi$, $R$ is much higher for larger $\mu$. 62
As shown by the error bars in Fig. 4.6, $R$ fluctuates from run to run, even for the same $\phi$. Such a fluctuation can be characterized by the relative fluctuation in $R$, defined here as $\delta R / R$, where $\delta R = \sqrt{\langle R^2 \rangle - \langle R \rangle^2}$ is the standard deviation of $R$ at the same $\phi$ for five runs. This relative fluctuation in $R$ is shown in Fig. 4.7 for different $\phi$ and $\mu$. Generally, fluctuations in both low and high $\mu$’s are bigger than that in medium $\mu$, which is furthermore shown in Table 4.2 by averaging $\delta R / R$ over all the $\phi$’s tested for each $\mu$. Bigger fluctuations at low and high $\mu$’s may be caused by variation in initial particles configurations, but in different ways. For low $\mu$, force chains are less stable when subject to perturbations, e.g. those from shear. This naturally leads to the high sensitivity to particle configurations. That is, built-up force networks could break down due to low $\mu$ and then follow a different pathway to create pressure. By contrast, for high $\mu$, the formation of the force networks depends dramatically on the initial configuration, resulting from a fairly low probability to break contacts once they are made. Hence, in both cases initial configurations contribute a lot to the large fluctuation in $R$. However, this cannot be avoided because complete particle scale density homogeneity is hardly possible to achieve.
Figure 4.7: Relative variation of Reynolds coefficients, $\delta R/R$, vs. packing fraction $\phi$ for different $\mu$’s, indicated by different colors and symbols.

Table 4.2: Reynolds coefficients variation for different $\mu$, averaged for each $\mu$ over all the densities tested.

<table>
<thead>
<tr>
<th>Particle</th>
<th>$\langle \delta R/R \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu = \mu_l$</td>
<td>0.21</td>
</tr>
<tr>
<td>$\mu = \mu_m$</td>
<td>0.07</td>
</tr>
<tr>
<td>$\mu = \mu_h$</td>
<td>0.36</td>
</tr>
</tbody>
</table>

4.3 Network Properties

The contact and force networks induced by shear also vary with $\mu$. One feature that distinguishes shear jamming from isotropic jamming is the anisotropy induced by shear, which is absent in isotropic jamming. Fabric and stress anisotropies, derived from the fabric and stress tensors to quantify anisotropy in contact and force networks, respectively, are investigated here at low and medium $\mu$. The case of $\mu = \mu_h$ is not studied for this particular purpose due to huge errors caused by the fine teeth on particle edges while applying our contact detection algorithm.

The fabric and stress anisotropies are shown for low $\mu$ (Fig. 4.8) and medium $\mu$ (Fig. 4.9). Two points are worth noting. First, both fabric and stress anisotropies show non-monotonic behavior with $f_{NR}$, the non-rattler fraction. This is consistent
with the observation that the majority of force chains first show up in the compression direction and then gradually percolate along every direction as shear continues. Second, the peak values of both fabric and stress anisotropy are notably higher for low $\mu$ than medium $\mu$. This corresponds to more straight force chains in the low $\mu$ system. However, the peak at low $\mu$ happens at fairly low $f_{NR}$, namely the very beginning of shear. At that stage, forces are relatively small and hence easily balanced, even with only two contacts.

To further understand the role friction plays in the contact network, the same
Figure 4.9: (a) Fabric anisotropy, and (b) stress anisotropy, vs. $f_{NR}$, the non-rattler fraction for systems with $\mu = 0.7$ at different packing fractions, indicated by different colors. Data shown here are within packing fractions ranging from 0.75 to 0.816.

Filter discussed in Chapter 3 is applied here to select the strong force network. Again, like in Chapter 3, ‘strong’ is defined as a contact force $f > \bar{f}$, where $\bar{f}$ is the mean force over all the contact forces at a certain step. Selecting contacts with only strong $f$ reveals that the backbone of force network that contributes the most to the pressure and stress build-up. An example of comparison of the fabric anisotropy between the total contact network and the strong one is shown in Fig. 4.10. The strong contact network obviously shows a higher anisotropy. Another point worth mentioning is that the fabric anisotropy at low $\mu$ is much higher than that at medium $\mu$. This would
imply more strong forces with smaller friction angle in the low $\mu$ case. However, this would be highly unstable under small perturbation, without more ‘weak’ contacts to stabilize.

### 4.4 Phase Diagram

By applying shear to various $\phi$, we can exploit the phase diagram for different $\mu$. With the photoelastic techniques, I can extract inter-particle contact forces [68], which can further determine the system $P$ and $\tau$ from the stress tensor, as discussed in Chapter 2. Because applying the inverse algorithm in [68] requires particle contacts, which are lacking for the $\mu_h$ case, data only for $\mu_l$ and $\mu_m$ is presented.

Fig. 4.11 (a) and (b) show phase diagrams for $\mu = \mu_l$ and $\mu = \mu_m$ systems, respectively. Of particular interest is the transition from fragile states (red crosses) to shear jammed states (green circles). The previous shear jamming phase diagram proposed by Bi et al. describes this transition line to decrease sharply after $\phi$ goes above $\phi_S$ and come to 0 as $\phi$ approaches $\phi_J$. However, from both $\mu = \mu_l$ and $\mu = \mu_m$, we can see that $\tau$ at the transition from fragile to shear jammed states almost stays the same for the $\phi$’s investigated. Therefore, based on this observation,
Figure 4.11: (a) Phase diagram for $\mu = \mu_l$ particles, depending on the packing fraction $\phi$ and the shear stress $\tau$, where red crosses indicate fragile states and green circles indicate shear jammed states. (b) The same phase diagram for $\mu = \mu_m$. (c) Revised shear jamming phase diagram for frictional granular materials, based on results in (a) and (b).

A revised shear jamming phase diagram is depicted in Fig. 4.11(c). In this revised phase diagram, the transition $\tau$ from fragile to shear jammed states stays almost the same for relatively small $\phi$ that is close to $\phi_S$, and starts to decrease rapidly to 0 as $\phi$ approaches $\phi_J$. 
4.5 Conclusions

In this chapter, I have studied the effect of friction on shear jamming by applying linear shear to systems with three different inter-particle μ’s. Shear jamming is still found for the smallest μ = 0.15 studied. However, as μ decreases, the amount of shear strain needed to reach shear jammed states increases for the same φ. A rescaled φ implies a universal behavior of γ_F and γ_{SJ} and reveals lower φ_S for higher μ. The pressure P also increases faster with γ as μ increases. The Reynolds coefficient R, characterizing increase in P with γ, shows higher fluctuations for both low and high μ, which can be potentially understood as being influenced by initial configurations. Detailed studies of the contact and force network reveal that there exist more straight chains in the ‘strong’ contact networks for lower μ.

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So far I have shown results concerning the mechanical response of granular materials under shear. By utilizing the experimental setup, particles have been shown to follow the applied affine shear strain until particle-particle collisions take place. Deviations from affineness are interesting because they reveal the static evolution of the system, though they may appear as random in a spatio-temporal description. The trimer mechanism discussed in Chapter 3 is a good example that explains the microscopic origins of shear jamming. In this chapter, I will look into particle displacements from a different point of view, namely diffusion.

Diffusion is commonly seen in a lot of systems, such as irreversible transport of atoms caused by random thermally-activated movement, brownian motion of particles suspended in a fluid, star motion within galaxies [75] and so on. Diffusion has been studied extensively in amorphous dynamical systems, e.g. colloids and glass forming materials. A commonly used quantity is the mean squared displacement (MSD). In addition to diffusion, dynamical heterogeneity associated with particle movements has also attracted much attention.

In the following part of this chapter, I study dynamics of granular systems with
different friction \( \mu \) in both cyclic shear and linear shear experiments. As a reminder, as shown in Chapter 4, three kinds of different \( \mu \) particles are used separately: \( \mu = 0.15 = \mu_l \), \( \mu = 0.7 = \mu_m \), and \( \mu = \mu_h > 1 \) (Table 4.1 in Chapter 4). In cyclic shear experiments, both translational and rotational diffusion behaviors are studied by tracking particles over all the cycles [70]. In linear shear experiments, I will define a diffusion matrix based on the non-affine displacements of particles. From this matrix, the diffusion anisotropy is studied. This is a rather small and much less studied quantity in colloidal and glassy systems due to the isotropic nature of diffusion in these systems.

5.1 Cyclic Shear

For a typical cyclic shear experiment, starting from a rectangular shape at \( \gamma = 0 \), the shear cell is sheared forward by several steps, each of which consists of small amplitude shear (\( \delta \gamma = 0.0045 \)), letting the system relax for six seconds afterwards, until a certain shear strain \( \gamma_{max} \) is achieved. Then the shear direction is reversed and the same number of shear steps are repeated to return to \( \gamma = 0 \). This completes one cycle. Usually the system is cyclically sheared by 500 cycles. At \( \gamma = 0 \) and \( \gamma = \gamma_{max} \) of each cycle, pictures are taken to record particle positions, orientations and contact forces. Three values are chosen for \( \gamma_{max} \): 0.027, 0.045, and 0.0675. A commonly used parameter to characterize the diffusive behavior is the mean squared displacement (rotation) for translation (rotational) movements, which depends on time. For cyclic shear here, I define time as the cycle number.

5.1.1 Displacement

From particle tracking, the mean squared displacement (MSD) is computed by:

\[
\langle \Delta r^2(t) \rangle = \langle (x(t_0 + t) - x(t_0))^2 + (y(t_0 + t) - y(t_0))^2 \rangle, \quad (5.1)
\]
Figura 5.1: (a) - (i): Mean squared displacement (MSD) data in the unit of the average particle diameter squared ($D^2$) for different types of particles under cyclic shear with different shear amplitudes $\gamma_{\text{max}}$, with different colors for different packing fraction $\phi$, plotted in log-log scale. Left: Teflon tape wrapped particles ($\mu = \mu_t$); middle: normal particles ($\mu = \mu_m$); right: gear particles ($\mu = \mu_h$). (a) - (c): $\gamma_{\text{max}} = 0.027$; (d) - (f): $\gamma_{\text{max}} = 0.045$; (g) - (i): $\gamma_{\text{max}} = 0.0675$. (j) - (l): corresponding displacement diffusion exponents, $\alpha_D$, with shear amplitudes indicated by different colors and symbols: red filled circles for $\gamma_{\text{max}} = 0.027$, green filled squares for $\gamma_{\text{max}} = 0.045$, and blue filled diamonds for $\gamma_{\text{max}} = 0.0675$. 

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where $x(t_0)$ and $y(t_0)$ are the positions of particles at time $t_0$ (time is defined as
the cycle number) and $\langle \cdots \rangle$ is an ensemble average over particles and all pairs of
steps for which the time interval $t$ is the same. Only particles that are at least $3.0$
times the average particle diameter away from all the shear walls are considered to
minimize influence from the boundaries.

Fig. 5.1 summarizes results for MSD for different $\phi$ and $\mu$. The relationship
between MSD and $t$ can be described as a power law: $\langle \Delta r^2(t) \rangle = D_0 t^{\alpha_D}$. $\alpha_D$, the
diffusion exponent, is 1 for a normal diffusion. A non-unity $\alpha_D$ indicates anomalous
diffusion, which has been observed in many systems, for instance, active matter and
systems of colloidal particles in bacterial suspensions [76]. If $\alpha_D > 1$, then it is called
super-diffusion. If $\alpha_D < 1$, then the particles undergo sub-diffusion. The MSD at
large $t$, e.g. Fig. 5.1(a), shows obvious deviation from a power law. This is due to
lack of statistics and $\langle \Delta r^2(t) \rangle$ at large $t$ is excluded while fitting the power law.

Fig. 5.1 (j) - (l) show the diffusion exponents as a function of $\phi$ and $\gamma_{\text{max}}$
for different $\mu$. Qualitatively, $\alpha_D$ behaves similarly as $\phi$ and $\gamma_{\text{max}}$ vary for different
$\mu$. $\gamma_{\text{max}}$ seems to have little effect on $\alpha_D$ for a given $\phi$. $\alpha_D$ has a value greater
than 1 at low $\phi$, which indicates super-diffusive behavior. This can be understood
as follows: while cyclic shear provides activation to the system, particles can move
rather freely without making strong contacts with their neighbor particles due to
a small amplitude of $\gamma_{\text{max}}$, and thus reveals a diffusion exponent greater than 1.
$\alpha_D$ almost remains the same until $\phi$ increases to a certain value and then starts to
decrease. The onset $\phi$’s where such a sharp turn of $\alpha_D$ for different $\mu$ systems are:
$\phi = 0.81$ for $\mu = \mu_t$, $\phi = 0.79$ for $\mu = \mu_m$, and $\phi = 0.74$ for $\mu = \mu_h$.

The onset $\phi$ presumably corresponds to the point when the system becomes glassy
to the activation of cyclic shear. That is, as $\phi$ increases, particles need to move co-
operatively due to the lack of free space. In order to verify our speculation that the
system becomes more glassy as $\phi$ increases, a further study on the dynamical het-
erogeneity is required. Widely investigated quantities like non-Gaussian parameter for the displacements probability distributions and susceptibilities of the four-point density correlation function are useful and reveal characteristic dynamical relaxation time and correlation length. However, these quantities are not available in this study mainly due to the lack of a large time scale. To obtain valid data on these, a time interval of at least 3 orders of magnitude is needed because glassy systems usually are associated with long relaxation times. Therefore, experiments with at least 1000 cycles for various \( \phi \)'s would be needed to possibly connect granular materials, which are athermal, to glass forming materials, which are thermal systems.

5.1.2 Rotation

Inter-particle friction impacts particle rotations once contacts form, potentially depending on the friction coefficient, \( \mu \). Hence, I apply similar analysis to the rotational diffusion of particles. The mean squared rotation (MSR) is defined as:

\[
\langle \Delta \theta^2(t) \rangle = \langle (\theta(t_0 + t) - \theta(t_0))^2 \rangle,
\]

where \( \theta(t_0) \) is the orientation of a particle at time \( t_0 \). The same ensemble average and the same set of particles, excluding ones that are too close to the shear walls, are chosen as in the MSD calculation. The rotational displacement, i.e. \( \Delta \theta(t) = \theta(t_0 + t) - \theta(t_0) \), is calculated in an integral form. That is,

\[
\Delta \theta(t) = \int_{t_0}^{t_0 + t} \Delta \theta(t') dt' = \sum_i \left( \theta(t_0 + t_i) - \theta(t_0 + t_{i-1}) \right),
\]

where \( t_i \)'s are the time series between \( t_0 \) and \( t_0 + t \). The reason why the integral form can be written as the sum of a series of rotational displacement over each cycle is because of the small amplitude of \( \gamma_{\text{max}} \).

Fig. 5.2 summarizes results for MSR for different \( \phi \) and \( \mu \). Similar to MSD, a diffusive behavior is observed for the rotation, namely, \( \langle \Delta \theta^2(t) \rangle = R_0 t^{\alpha_R} \). Fig. 5.2
Figure 5.2: (a) - (i): Mean squared rotation (MSR) data in the unit of radian squared for different types of particles under cyclic shear with different shear amplitudes $\gamma_{\text{max}}$, with different colors for different packing fraction $\phi$, plotted in log-log scale. Left: Teflon tape wrapped particles ($\mu = \mu_l$); middle: normal particles ($\mu = \mu_m$); right: gear particles ($\mu = \mu_h$). (a) - (c): $\gamma_{\text{max}} = 0.027$; (d) - (f): $\gamma_{\text{max}} = 0.045$; (g) - (i): $\gamma_{\text{max}} = 0.0675$. (j) - (l): corresponding rotation diffusion exponents, $\alpha_R$, with shear amplitudes indicated by different colors and symbols: red filled circles for $\gamma_{\text{max}} = 0.027$, green filled squares for $\gamma_{\text{max}} = 0.045$, and blue filled diamonds for $\gamma_{\text{max}} = 0.0675$. 
Figure 5.3: The self part of the von Hove function $G_s(\Delta \theta, t)$ for different $\phi$ and $\mu$, with $\gamma_{max} = 0.045$. (a) - (c): Teflon tape wrapped particles ($\mu = \mu_l$); (d) - (f): normal particles ($\mu = \mu_m$); (g) - (i): gear particles ($\mu = \mu_h$). Here $\Delta \theta$ is rescaled by the standard deviation $\sigma$ at each $t$. Three $\phi$'s are selected for each $\mu$, as indicated on each sub-figure. A normal distribution, namely, a Gaussian distribution with the mean to be 0 and the standard deviation to be 1 is also plotted as reference (red line).

(j) - (l) present the rotational diffusion exponent $\alpha_R$. The behavior of $\alpha_R$ shows a certain resemblance with that of $\alpha_D$, e.g., $\alpha_D$ also seems to be weakly affected by $\gamma_{max}$. However, friction has an impact on $\alpha_R$. For $\mu = \mu_m$, $\alpha_R$ again remains almost the same until $\phi$ is greater than 0.79, similarly to the behavior of $\alpha_D$. Nevertheless, for $\mu = \mu_l$, $\alpha_R$ remains almost constant for all the $\phi$'s. Different behaviors of $\alpha_R$ for $\mu_l$ and $\mu_m$ may suggest a decoupling between the translational diffusion and the
rational diffusion as $\mu$ decreases. As for $\mu = \mu_h$, the data scatters much more than the other two $\mu$’s, with no clear trend as $\phi$ increases.

The self part of the von Hove function is commonly used to study the probability distribution of particle displacements in glassy and supercooled liquids systems [77]. To study the statistics of particle rotations, a similar function is calculated as:

$$G_s(\Delta \theta, t) = \frac{1}{N} \sum_{j=1}^{N} \langle \delta(\Delta \theta - (\theta(t) - \theta(0))) \rangle,$$  \hspace{1cm} (5.4)

where $N$ is the total number of particles, $\delta$ is the Dirac delta function and $\langle \cdots \rangle$ is an ensemble average over all the starting steps. Typical results are shown in Fig. 5.3 for all three $\mu$’s, each with three representative $\phi$’s. For a normal diffusion and in thermal ballistic transport, $G_s(\Delta \theta, t)$ is a Gaussian distribution. However, Fig. 5.3 clearly shows that is not the case here. For $\mu = \mu_m$, the distribution remains the same functional form as $t$ increases. The functional form changes with $\phi$, with the peak of $G_s(\Delta \theta, t)$ shifting to a lower value and the shape of the function going from very non-Gaussian to increasingly Gaussian as $\phi$ gets larger. In contrast, for both $\mu_l$ and $\mu_h$, the functional form of $G_s(\Delta \theta, t)$ varies with $t$ at small $t$ and approaches an asymptotic form as $t$ increases. Meanwhile, the functional form at large $t$ seems not to vary with $\phi$.

Differences in the evolution of $G_s(\Delta \theta, t)$ vs. $t$ for various $\mu$’s coincide with the behavior of $\alpha_R$. Clearly inter-particle friction makes a difference in the rotational diffusion. It will be useful to incorporate friction and develop a statistical model accounting for the distribution of $\Delta \theta$. Both $G_s(\Delta \theta, t)$ and $\alpha_R$ show dependence on $\mu$, hence, another future direction is to study frictional systems with more $\mu$, which may be less time-consuming for simulation work.
5.2 Linear Shear

For linear shear, results shown below are obtained from the same experiments described in Chapter 4. Unlike cyclic shear, there is no procedure to bring particles back to their original places in linear shear. Diffusion studied in the previous section characterizes how much particles deviate from where they would be if there were no particle collisions. Therefore, following the same spirit, I define a diffusion matrix in 2D based on the non-affine displacements as follows:

\[
MSD(\gamma) = \langle \begin{pmatrix}
\Delta x(\gamma) \cdot \Delta x(\gamma) & \Delta x(\gamma) \cdot \Delta y(\gamma) \\
\Delta y(\gamma) \cdot \Delta x(\gamma) & \Delta y(\gamma) \cdot \Delta y(\gamma)
\end{pmatrix}\rangle,
\]

where \(\Delta x(\gamma)\) and \(\Delta y(\gamma)\) are the x and y components of the non-affine displacements at shear strain \(\gamma\) compared to \(\gamma = 0\), and \(\langle \cdots \rangle\) is an average over particles. Again the outer two layers of particles of the packing are excluded in the calculation. The trace of this matrix gives the mean squared non-affine displacement. Due to the symmetric nature of this matrix, there will always be two eigenvalues and eigenvectors. Denoting the eigenvalues as \(d_1\) and \(d_2\), the MSD anisotropy is defined as \(|d_1 - d_2|/(d_1 + d_2)\).

Fig. 5.4(a) shows typical examples of the MSD anisotropy for \(\mu = \mu_m\) systems with different packing fractions \(\phi\). The MSD anisotropy starts to increase rapidly at the beginning of shear, soon (of order of 0.1 for shear strain \(\gamma\)) reaching a maximum, which is approximately 0.85 for all \(\phi\). Then the anisotropy decreases approximately linearly with \(\gamma\) until a relatively small value. That is, as \(\gamma\) increases, the diffusion process becomes more and more isotropic. In other words, a granular system undergoes a transient stage before it reaches isotropic diffusion/non-affine movements under linear shear. Similar results are observed for the other two \(\mu\) systems.

In order to characterize the transient stage, I use a linear regression to fit a line between the MSD anisotropy and \(\gamma\) after selecting the decay region. Fig. 5.4(b) shows the same data from Fig. 5.4(a) with \(\phi = 0.794\), with the selected decay region.
Figure 5.4: Decay of the MSD anisotropy with shear strain $\gamma$. (a) A few examples of the change of the MSD anisotropy vs. $\gamma$, with different colors and symbols indicating different packing fractions $\phi$. These are samples from systems with $\mu = \mu_m$. Similar trends of the MSD anisotropy vs. $\gamma$ for $\mu = \mu_l$ and $\mu = \mu_h$ are observed (not shown here). (b) An example from (a) ($\phi = 0.794$) to illustrate the region chosen for the linear fit and the slope of the line from the fit. (c) The MSD anisotropy decay speed vs. packing fraction $\phi$, averaged over 5 runs for each $\phi$, for different $\mu$, indicated by different colors and symbols.
and the resulting slope of the fitted line. The decay speed, defined as the absolute value of the slope, depends on $\phi$, as plotted in Fig. 5.4(c). For any $\mu$, the decay speed remains very small (of order 0.1) at low $\phi$ until $\phi$ increases to a certain value. As $\phi$ goes above this value, the decay speed increases dramatically. From Fig. 5.4(c), the onset $\phi$ for the decay speed to increase rapidly is approximately: 0.81 for $\mu = \mu_l$, 0.79 for $\mu = \mu_m$, and 0.74 for $\mu = \mu_h$. Interestingly, this behavior of the decay speed is reminiscent of that of $\alpha_D$ as discussed in Section 5.1.1, where $\alpha_D$ remains almost constant at low $\phi$ and shows a sharp turn after an onset $\phi$. Even more interestingly, the onset $\phi$’s for different $\mu$ shown in the decay speed seem to coincide with the ones displayed by the behavior of $\alpha_D$. This coincidence suggests a possible connection between the transient stage, e.g. the MSD anisotropy decay speed, and the structural properties that are usually probed at a large time scale, i.e., particles diffusion. The underlying reason needs to be further investigated, which could also help understand glassy systems. Furthermore, this points out another direction for studying glassy systems via measurements at the transient state. These measurements take much less time, which provides an advantage over those taken at the steady state for a much longer time.

5.3 Conclusions

To summarize, I have studied particle diffusion in both cyclic shear and linear shear experiments. In cyclic shear, particles show abnormal diffusion with a $\phi$-dependent diffusion exponent in both mean squared displacement (MSD) and mean squared rotation (MSR) measurements. $\alpha_D$, the diffusion exponent for MSD, remains the same at low $\phi$ and decreases above a certain $\phi$ as $\phi$ approaches the isotropic jamming point $\phi_J$. In linear shear, I define a diffusion matrix based on the non-affine displacements. The MSD anisotropy shows an approximately linear decrease with shear strain $\gamma$ at the beginning of shear, indicating diffusion/non-affine motion becomes more and...
more isotropic. The MSD anisotropy decay speed, which is the absolute value of the slope for the linear decrease part, shows surprisingly similar dependence on $\phi$, for various $\mu$ systems. This decay speed starts to increase dramatically until $\phi$ reaches a certain value as it approaches $\phi_J$ from below. Presumably, the onset $\phi$ for $\alpha_D$ and the $\phi$ where the decay speed shows a dramatic change is the point when the system starts to become glassy, which would however require further experiments to verify. The observation in the linear shear provides a novel angle to characterizing non-affine displacements and to study glassy systems with a much shorter time required.
So far, I have only considered the simplest shape in 2D, i.e. discs, to model granular systems. Systems composed of disks (in 2D) or spheres (in 3D) under shear have been studied extensively in theory and experiments, including simulations [78, 16, 18, 36, 68, 79, 31, 80, 35]. Though simple and able to capture important features of granular systems, disk/sphere models are often different from real situations, i.e., particles have an anisotropic or even irregular shape. Much is less known for this type of systems.

One of the simplest anisotropic shapes is an ellipse. There have been studies on ellipses, with comparisons to disks, i.e., jamming transitions and dynamical properties, both in experiments and simulations [81, 82, 83, 84]. Most of these studies either focus on systems above jamming or consider dynamics. Therefore, it is necessary to test shear jamming in a system of ellipses.

In this chapter, I will use particles of elliptical shape, made of photoelastic materials, to probe response of granular system with an anisotropic shape to quasi-static
linear shear. In order to investigate the difference for the shear response between disk and ellipse systems, I probe structural changes in the ellipse system and, where appropriate, contrast them with disks. Specifically, I look at the probability distribution function (PDF) and changes of orientations of ellipses, denoted as \( \theta_e \) in the following, and apply Voronoï tessellation to the packing, with results shown and discussed below. Furthermore, I test shear jamming properties in elliptical granular systems.

The system consists of approximately 3000 monodispersed elliptical particles, whose major and minor axes are 1.04 cm and 0.57 cm, respectively. The packing fraction, \( \phi \), ranges from 0.76 to 0.85 and is controlled by adding or removing particles. The same quasi-static linear shear procedure as described in Chapter 4 is followed to apply a total shear strain \( \gamma \) up to 0.27.

6.1 Particle Orientations

When computing the probability distribution function of the orientations of ellipses, only ellipses whose distances to the nearest boundary are twice or more the minor axis are taken into consideration to minimize the boundary effect. After eliminating boundary particles, about 2500 particles are left for the calculation, which still gives reliable statistical results.

For ease of plotting, \( \theta_e \) is first confined in the range \( (0^\circ, 180^\circ) \) and then extended to \( (0^\circ, 360^\circ) \) by adding 180° to the original values. To better illustrate the orientations of particles and shear, the coordinate system on which all the geometric quantities are computed is shown in Fig. 6.1. Results from a few selected \( \gamma \) are shown in Fig. 6.2. Note that at \( \gamma = 0 \) in Fig. 6.2(a), there are more ellipses oriented around 80°, while supposedly there would be no preferred orientations if particles were oriented randomly. The main reason for this is that in order to achieve a stress free state at a relatively high \( \phi \), particles tend to align with their neighbors, which hence creates
Figure 6.1: The sketch of the experiment setup, with the coordinate system used to determine particle centers and orientations. The red arrows indicate the direction of shear. Based on the orientation detected, each particle is assigned with a unit vector $\vec{v} = (v_x, v_y)$, whose direction is the same as the particle orientation.

Local order. More particles orient around $80^\circ$ in this specific example, while this value varies in other runs. However, such a built-in order does not affect the final conclusion, as seen in the following.

As $\gamma$ increases, we can clearly see in Fig. 6.2 that: first, the distribution remains non-uniform; second, the most probable $\theta_e$ changes from $\sim 80^\circ$ at $\gamma = 0$ to $\sim 110^\circ$ with a slightly higher probability at $\gamma = 0.15$, and then stays around the same value for the rest of shear. The first feature indicates that shear induces or keeps a preferred direction in an ellipse system. The second feature indicates that the system reaches a steady state. Such a feature is reminiscent of the work by Börzsönyi et al., who showed that a granular system of elongated particles tended to orient at a certain angle with the streamline of shear, regardless of the shear rate [84]. Furthermore, both features show up for all the other densities tested.

Linear shear can be decomposed into two actions: a pure shear with compression in one direction and dilation in the perpendicular one, and rotation. The amount of rotation associated with simple shear is given by $\tan^{-1}(\gamma/2)$, which in our case is no larger than $\tan^{-1}(0.27/2) = 7.7^\circ$. From Fig. 6.2, we clearly see that the change of the preferred $\theta_e$ is more than $15^\circ$. Therefore, such a change cannot only be induced
Figure 6.2: The probability distribution function of the orientation of ellipses with packing fraction $\phi = 0.847$, excluding particles that are close to the boundary at different strain $\gamma$: (a) $\gamma = 0$, (b) $\gamma = 0.0513$, (c) $\gamma = 0.1026$, (d) $\gamma = 0.1539$, (e) $\gamma = 0.2052$, and (f) $\gamma = 0.2565$. In the figures, the orientations are first fixed to the range $[0^\circ, 180^\circ]$ and then duplicated by adding $180^\circ$ to have a range in $[0^\circ, 360^\circ]$.

by the rotation associated with shear. Note that an ellipse is more stable if the forces it bears are mainly perpendicular to its major axis. Combining this with the fact that shear induces force anisotropy with larger forces mainly in the compression direction, particles are naturally expected to align their major axis perpendicular to the compression direction. This expectation coincides with our observation that the most probable $\theta_\epsilon$ is around $110^\circ$, which is very close to the perpendicular direction of compression direction ($45^\circ - tan^{-1}(\gamma/2) + 90^\circ = 135^\circ - tan^{-1}(\gamma)$, which is $120^\circ$ for $\gamma_{\text{max}} = 0.27$).

Assigning two values to one particle, like showing the PDF of $\theta_\epsilon$ above, is not mathematically convenient and creates an ambiguity. To better describe the collective behavior of particle orientations, e.g. how ordered the alignments are and
Figure 6.3: Nematic order parameter (a) and the preferred orientation $\theta_{ep}$ (b), calculated from the nematic matrix $Q$ (Equation 6.1), plotted vs. shear strain $\gamma$ for different packing fractions $\phi$, indicated by different colors and symbols. Also plotted in (b) are the stretched exponential fit in solid lines (Equation 6.2).

what the preferred alignment direction is, and remove the ambiguity of defining the orientation, the nematic order matrix $Q$, which is a commonly used tensor in the liquid crystal community [85], is used:

$$Q = \left\langle \begin{pmatrix} n_x n_x - \frac{1}{2} & n_x n_y \\ n_x n_y & n_y n_y - \frac{1}{2} \end{pmatrix} \right\rangle,$$

(6.1)

where $n_x$ and $n_y$ are the $x$ and $y$ components of the unit vector $\vec{n}$ aligned with the major axis of each particle and $\langle \cdots \rangle$ is an average over all particles excluding ones that are too close to the boundary. The unit vector is given by $\vec{n} = (n_x, n_y) = (\cos \theta_e, \sin \theta_e)$, e.g. Fig. 6.1. $Q$ is a symmetric matrix with 0 trace. That is, $Q$ always
has two equal and opposite eigenvalues. The nematic order, $S$, is defined as twice the positive eigenvalue, characterizing the order of alignment of a packing of rod shape particles. The larger $S$ is, the more aligned particles are. $S$ is in the range of $[0, 1]$. The preferred alignment direction, $\theta_{ep}$, is the same as the direction of the eigenvector corresponding to the positive eigenvalue. The definition of $Q$ ensures that $S$ and $\theta_{ep}$ are invariant under rotation, e.g., these quantities are not affected by switching the direction of $\vec{n}$ to $-\vec{n}$, or equivalently, adding $\pi$ to $\theta_e$.

Fig. 6.3 shows the evolution of the nematic order $S$ and the preferred direction $\theta_{ep}$ as a function of shear strain $\gamma$ for different packing fractions $\phi$. Starting from a very low value, $S$ starts to grow after a certain amount of strain (Fig. 6.3(a)). Such an increase in $S$ clearly indicates particle alignment during shear. Mechanically, particles are more stable when contacts are closer to their minor axes. This mechanical preference shows up as more and more particles make contacts due to shear and results in an emergent nematic order. As for the preferred direction $\theta_{ep}$ (Fig. 6.3(b)), the starting point varies a lot with $\phi$. However, this starting point is less important, because $S$ at $\gamma = 0$ is rather small. Interestingly enough, $\theta_{ep}$ seems to approach a certain value asymptotically as $\gamma$ increases, which is consistent with the evolution of the PDF of $\theta_e$ discussed above.

To further test the asymptotic behavior of $\theta_{ep}$, its relationship with $\gamma$ is fitted using a stretched exponential function:

$$\theta_{ep}(\gamma) = \theta_{e0} - (\theta_{e0} - \theta_{ep}(0)) \cdot e^{\exp\left(-\left(\frac{\gamma}{\gamma_0}\right)^\alpha\right)}, \quad (6.2)$$

where $\theta_{ep}(0)$ is the value of $\theta_{ep}$ at $\gamma = 0$ and $\theta_{e0}$, $\gamma_0$ and $\alpha$ are the fitting parameters. Fig. 6.4(b) also plots the fit in solid lines, which clearly shows an excellent agreement between the data and the fit.

Fig. 6.4(a) shows $\theta_{e0}$ as a function of packing fraction $\phi$. It seems that $\theta_{e0}$ changes little for different $\phi$, with variances of only a few degrees. Averaging over all $\theta_{e0}$
Figure 6.4: The packing fraction ($\phi$) dependence for the fitting parameters in the stretched exponential function (Equation 6.2): (a) $\theta_{e0}$ and (b) $\gamma_0$. Each data point is averaged over 5 runs. In (a), the red dashed line indicates a value of 123°, which is the average of $\theta_{e0}$ over all the data.

reveals a value of 123°, shown as a red dashed line in Fig. 6.4(a). The independence of $\theta_{e0}$ on $\phi$ indicates that this property may be caused purely due to geometry, i.e. the aspect ratio. The characteristic relaxation strain, $\gamma_0$, shows weak yet non-monotonic dependence on $\phi$, as shown in Fig. 6.4(b). Error bars, calculated as the standard deviation, are relatively large when compared to the values of $\gamma_0$. Nevertheless, in general, Fig. 6.4(b) shows that $\gamma_0$ is of order 0.1. This provides an estimate for the transient stage, which may be useful in future research if this transient region needs to be avoided.
6.2 Local Packing Fraction

To further verify the structural change of the ellipse system under shear, a Voronoï tessellation is applied to the packing. In this approach, I use the distance transformation tool in Matlab to determine a Voronoï tessellation associated with a particle, in which the distance of any point to the surface of that particle is less than that to any other particle [86]. In order to prevent particle intersections, which is possible due to imprecision of the particle detection and compression of particles at larger shear strains, the detected ellipses are first shrunk by 1/10 in length in all directions while maintaining the aspect ratio the same. Then a watershed method separates all the particle with boundaries containing the Voronoï tessellation associated with each of them. Fig. 6.5 shows an example of finding the tessellation from the original image.

Following the same procedure as in Section 6.1 to minimize boundary effects, the results for Voronoï areas are shown in Fig. 6.6. Fig. 6.6(a) shows the evolution of the PDF of the Voronoï area, $A_{vor}$, with shear. The peak value of the PDF of $A_{vor}$ shifts to a lower value as $\gamma$ increases. In comparison, Ren et al. reported that
this PDF did not change during shear for a disk system \[87\]. In addition, Aste \textit{et al.} showed an invariant Gamma distribution of the Voronoï volume in static granular spheres of different packing fraction by rescaling the Voronoï volume \[80\]. Here I apply the same rescaling: \( A_{\text{rescaled}} = (Avoro - A_{\text{min}}) / (\langle Avoro \rangle - A_{\text{min}}) \), where \( A_{\text{min}} \) is the minimum and chosen to be 1.048 times the actual area of an ellipse. Assuming the data to be characterized by the Gamma distribution, given by

\[
P(A_{\text{rescaled}}) = \frac{1}{\Gamma(k)\theta^k} A_{\text{rescaled}}^{k-1} e^{-A_{\text{rescaled}}/\theta},
\]

(6.3)

\( k \) and \( \theta \) can be determined by the mean \((k\theta)\) and variance \((k\theta^2)\). One thing to note is that due to the rescaling, the mean is always 1, namely, \( k\theta = 1 \).

An example of the Gamma distribution fit is shown in Fig. 6.6(b) for \( \gamma = 0 \). Since \( k\theta \) is fixed regardless of \( \gamma \), we only look at \( k \) here, plotted against \( \gamma \) as shown in Fig. 6.6(c). Starting from a value around 8, \( k \) stays the same for small \( \gamma \) and then gradually decreases as \( \gamma \) increases. The skewness of the Gamma distribution is proportional to \( 1/\sqrt{k} \), hence the PDF of \( Avoro \) becomes more and more asymmetric as \( \gamma \) increases.

6.3 Shear Jamming

Apart from the structural evolution induced by shear, the mechanical response is also interesting to look at, especially the shear jamming transition for frictional granular systems.

Shear jamming is still observed in the case of ellipses, and that is qualitatively similar to what is observed for disks. According to the simulations \[88\], the isotropic jamming point, \( \phi_J \), for a frictionless bidisperse ellipse system with an aspect ratio 1.82\((= 1.04/0.57)\) is between 0.885 and 0.89. The densities tested are all well below this value. Typical results from an example of \( \phi = 0.847 \) are shown in Fig. 6.7.
Figure 6.6: (a) Probability distribution function (PDF) of the Voronoi area of ellipses in the unit of the area of an ellipse, $\text{Avoro/Aelp}$, from the same experiment in Fig. 6.2, as a function of shear strain $\gamma$, indicated by different colors. The inset shows the color bar for $\gamma$. (b) The Gamma distribution fit (red line) to the original data (blue crosses) at $\gamma = 0$ for the rescaled Voronoi area: $A_{\text{rescaled}} = (A - A_{\text{min}})/\langle A \rangle - A_{\text{min}}$. (c) The evolution of $k$ from the Gamma distribution fit as $\gamma$ increases.

Starting from a completely stress-free state, as shown in Fig. 6.7(a), where no particle is bearing any force, the system gradually comes to a fragile state, where particles form a force network, or force chains, mainly in the compression direction, as shown in Fig. 6.7(b) [36, 35]. Such a special state is mechanically stable; however, it cannot sustain more than a small stress if the shear is reversed. This feature distinguishes itself from a jammed state, where the system can sustain stress from any direction. As $\gamma$ further increases, force chains in the compression direction bend and make extra contacts, and eventually percolate all over the system, bringing the system to a jammed state, as shown in Fig. 6.7(c).

Quantitatively, the system pressure, $P$, is calculated by the $G^2$ method. Fig. 6.8 shows typical $P$ response at different packing fractions $\phi$. We clearly see that $P$ does not increase until $\gamma$ reaches a certain value, especially for lower $\phi$. Based on the
Figure 6.7: Three snapshots of polarized images from one shear experiment \( (\phi = 0.847) \) showing that the system undergoes transitions from (a) unjammed to (b) fragile and eventually to (c) shear jammed states. The corresponding strains from (a) to (c) are \( \gamma = 0, 0.027, 0.135 \).
Figure 6.8: Representative pressure ($P$) response to shear strain $\gamma$ at different packing fraction $\phi$, indicated by different colors and symbols. $P$ is calculated via the $G^2$ method, which has an arbitrary unit. The dashed line indicates the point from which $P$ starts to deviate from zero. This point defines the onset of fragile states, $\gamma_F$.

Figure 6.9: (a) The onset of fragile states, $\gamma_F$, averaged over 5 runs, plotted against the packing fraction $\phi$. (b) $\log_{10}(\gamma_F)$, plotted against the distance to the isotropic jamming point of frictionless ellipses with the same aspect ratio, $\log_{10}(\phi_J - \phi)$. $\phi_J$ is chosen to be 0.888 according to [88].
force percolation argument, the fragile state corresponds to force network formation connecting 2 or 3 of the shear walls but not all 4 and these networks normally appear along the compression direction of shear [35]. Once these networks form, they will be compressed more as $\gamma$ increases. Hence, we can define the point from which $P$ starts to grow dramatically as the onset for fragile states, denoted as $\gamma_F$.

Fig. 6.9(a) presents the dependence of $\gamma_F$ on $\phi$. Similar to that observed in disk systems (discussed in Chapter 4), $\gamma_F$ decreases monotonically with $\phi$. A further test of the dependence of $\gamma_F$ on $\phi$ reveals that $\gamma_F \sim (\phi_J - \phi)^\alpha$, as shown in Fig. 6.9(b), where $\phi_J$ is the isotropic jamming point for a system of ellipses with an aspect ratio of 1.82. $\phi_J$ is chosen to be 0.888 according to [88]. A linear fit between $\log_{10}(\gamma_F)$ and $\log_{10}(\phi_J - \phi)$ reveals $\alpha \approx -1.7$.

In addition, the best fit reveals that $P$ does not follow the quadratic relationship with $\gamma$ after $\gamma > \gamma_F$, as observed for disk systems. Therefore, changing particle shapes from disks to anisotropic shapes like ellipses also has impacts on the mechanical response, which is left for further investigation.

Determining the onset for shear jamming transition requires particle contact numbers, which is not accessible at the current stage due to difficulties in processing ‘P’ images. Slat edges significantly impact the image intensity, resulting in errors while computing $G^2$ at the possible contact points. This kind of problem exists as well for disk systems. However, disks investigated in previous study have much more pixels than ellipses and hence contacts detection is less affected by slat edges. For future work, it would be better if the resolution on the particle scale were improved so that accurate contacts could be detected.

### 6.4 Conclusions

In summary, I have presented structural evolution and mechanical response of a granular system composed of ellipses under linear shear. Particles tend to align in a
certain direction asymptotically, i.e., approximately 120° referring to Fig. 6.1, regardless of the packing fraction. This alignment shows up in the probability distribution function of particle orientations and an increase of the nematic order parameter $S$ calculated from the nematic matrix $Q$. Furthermore, analysis on the Voronoï cell reveals a shift of the most probable value to a smaller value, which is consistent with the particle orientation alignment observed earlier. Shear jamming is still observed in the ellipse system, with the onset for fragile states decreasing as a power law as $\phi_J - \phi$ approaches 0. The pressure $P$ seems to increase with $\gamma$ in a law other than quadratic, which indicates possible change in mechanical response by introducing anisotropic shapes.
7

Conclusions and Outlook

7.1 Summary

In this thesis, I have presented a comprehensive study of the response to shear of granular materials with various particle properties. By utilizing a novel setup suppressing shear bands, I have applied quasi-static linear shear and cyclic shear to granular systems composed of photoelastic particles. The photoelastic particles enable tracking information like particle positions, orientations and particle-scale forces. Properties for these particles, including inter-particle friction and particle shapes, are varied to study their effects on the system response to shear. Major results are summarized below:

1. By applying linear shear to systems of particles with $\mu = 0.7$ within $\phi_S < \phi < \phi_J$, I have proposed the microscopic mechanisms accounting for shear jamming for frictional granular grains: trimers and branches. Trimers oriented close to the compression direction tend to bend under shear. This bending process pushes the center particle of a trimer out faster in the dilation direction than the applied shear strain, which provides a more effective mechanism to create
new contacts for the center particle. The geometric measurement $O$ of trimers that form the force networks at shear jamming show collective evolution with shear strain. In addition, $O$ values at the shear jamming onset are independent of $\phi$, which strengthens the usefulness of $O$ to serve as an order parameter. Furthermore, $O$ selects particles that contribute the most to the build-up of pressure during shear jamming. Branches provide a second mechanism to increase particle contacts and redirect orientations of force chains.

2. Systems of particles with different friction show shear jamming still exists even when inter-particle friction coefficient $\mu$ is as low as 0.15. Friction does affect some aspects of shear jamming: first, $\phi_S$ increases as $\mu$ decreases; second, force networks induced by shear show larger anisotropy for lower friction systems; third, both low and high friction systems show large variance in the pressure response. However, the onset shear strain for shear jamming collapses into one curve for different $\mu$’s after rescaling $\phi$, indicating a universal behavior for shear jamming for frictional systems regardless of friction. Both large and small $\mu$ systems show high variance in the pressure response.

3. The dynamics of particles with different $\mu$ show abnormal diffusion under cyclic shear. The translational diffusion exponents exhibit a transition as $\phi$ varies, with the onset $\phi$ depending on $\mu$. The rotational diffusion exponents show different behavior as $\mu$ changes, indicating a possible decoupling of translation and rotation. Under linear shear, the non-affine displacements are anisotropic, with the anisotropy increasing rapidly for small $\gamma$, decaying as $\gamma$ increases, and then remaining at a relatively small value. The speed of such a decay shows an almost discontinuous transition as $\phi$ varies. Interestingly the onset $\phi$ for this anisotropy decay speed coincides well with the ones observed for the translational diffusion exponents.
4. Granular systems of ellipses undergo structural evolution under shear. These structural changes include changes of the PDF of the Voronoï area distribution as $\gamma$ increases, which is absent in the disk systems [87], and ellipse alignment induced by shear, which leads to an increase of the nematic order and an emergence of a preferred orientation. This preferred orientation seems to be independent of $\phi$. Shear jamming is still observed for ellipse systems. However, the pressure increase with $\gamma$ seems not to follow the quadratic relationship with $\gamma$, as reported in the disk systems [43].

7.2 Future Outlook

The above findings point towards possible future research directions as follows:

1. With the mechanisms enabling shear jamming for frictional granular systems, where the stability of trimers and the maximum bending angle depend particularly on friction, one obvious direction is to extend the analysis of these mechanisms to predict shear jamming for different $\mu$. One proposition is that $\phi$ determines how fast trimer particles that form the force networks at shear jamming make contacts and $\mu$ constrains the possible distribution of trimer bending angles with a upper cut-off. Results derived from this proposition can be compared with those in Chapter 4.

2. Analysis also shows that trimer bending provides a faster extension in the dilation direction than the actual affine shear strain field, which contributes to the build-up of force chains in the dilation direction and furthermore the formation of rigid force and contact networks as shear strain increases. Therefore we can apply a new type of shear, which is composed of compression in one direction and dilation in the perpendicular one with a constant dilation speed of the area. This type of shear shares a similar spirit with pure shear, except for
non-conservation of the area. This shear protocol can be accomplished with a newly built biaxial setup in our lab, whose four walls can move independently. Then by varying the dilation speed, we can study the competition mechanism between trimer bending and dilation.

3. Trimer structures presumably are not unique to shear. Stabilized by friction, they could also exist in systems undergoing other types of deformation, as long as compression in a certain direction is present. Therefore it will be interesting to apply analysis using trimers to other processes, such as uni-axial and bi-axial compression.

4. Baity-Jesi et al. have shown dependence of the onset $\gamma$ for shear jamming on the system size, i.e. the number of particles, in a frictionless granular system [42]. It is thus useful to test this dependence in frictional systems. Preliminary experimental data show similar results for granular systems composed of 1000 and 3000 particles. By increasing particle diameters, the number of particles with the same $\phi$ can be decreased by an order of magnitude to $N \sim 100$. Possible quantities worth looking into include the onset $\gamma$ for shear jamming, fluctuations, and the pressure response. From these results, we can further study the statistical properties of granular materials, e.g. testing or constructing ensemble descriptions.
Bibliography


Biography

Dong Wang was born on August 14, 1991 in Lu’an, Anhui Province, China. He earned his Bachelor of Science degree in Applied Physics from University of Science and Technology of China in 2012. He then pursued his Doctor of Philosophy degree in Department of Physics at Duke University. Since 2013 spring, he joined Prof. Robert Behringer’s lab to study granular materials, specifically on the shear response of granular systems with different particle properties.

During his time at Duke, Dong has been honored with the Research Triangle MRSEC Fellowship, awarded by the Research Triangle MRSEC funded by NSF. He has served as session chair at the 69th Annual Meeting of the APS Division of Fluid Dynamics in 2016. He was invited to present his work on understanding the microscopic origins of shear jamming at APS March Meeting 2017. He has three publications on the subject of shearing granular materials [89, 90, 91, 92].