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Shape effects on time-scale divergence at athermal jamming transition of frictionless non-spherical particles

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HIGHLIGHTS

- We numerically discover a time-scale divergence at athermal jamming transition for various nonspherical particles.
- Two main shape effects, elongation and roundness, are systematically investigated.
- Plastic behaviors of over-jammed packings can evaluate the robustness of jamming states for different shapes.

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ABSTRACT

The critical behaviors of a granular system at the jamming transition have been extensively studied from both mechanical and thermodynamic perspectives. In this work, we numerically investigate the jamming behaviors of a variety of frictionless non-spherical particles, including spherocylinder, ellipsoid, spherotetrahedron and spherocube. In particular, for a given particle shape, a series of random configurations at different fixed densities are generated and relaxed to minimize interparticle overlaps using the relaxation algorithm. We find that as the jamming point (i.e., point J) is approached, the number of iteration steps (defined as the "time-scale" for our systems) required to completely relax the interparticle overlaps exhibits a clear power-law divergence. The dependence of the detailed mathematical form of the power-law divergence on particle shapes is systematically investigated and elucidated, which suggests that the shape effects can be generally categorized as elongation and roundness. Importantly, we show the jamming transition density can be accurately determined from the analysis of time-scale divergence for different non-spherical shapes, and the obtained values agree very well with corresponding ones reported in literature. Moreover, we study the plastic behaviors of over-jammed packings of different particles under a compression–expansion procedure and find that the jamming of ellipsoid is much more robust than other non-spherical particles. This work offers an alternative approximate procedure besides conventional packing algorithms for studying athermal jamming transition in granular system of frictionless non-spherical particles.

1. Introduction

Jamming transition, which occurs when a disordered system transits from a liquid-like to a solid-like state, has been extensively studied for many years [1–6]. A unified framework associated with the jamming phase diagram was introduced by Liu et al. to combine density, applied shear stress, and temperature all together [7–9]. The critical behaviors at point J,

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the athermal transition point without applied shear stress in the jamming diagram, have been demonstrated from both mechanical [9–12] and thermodynamic [13–18] perspectives. Roughly speaking, conventional methodologies are based on existing reference systems, or packings in other words, subjected to mechanical or thermal fluctuation. Besides, the relationship among the point J, the random close packing (RCP), and the maximally random jammed (MRJ) state is still an open question, [1–3,5,19,20] especially when it comes to non-spherical particles such as polyhedra [21–25]. In the following, this critical state is termed ϕ_J without distinction.

To generate jammed packings from initial gas-like configurations, O'Hern and his colleagues developed a quasi-static compression protocol for soft particles, avoiding any thermal equilibrium [6,8,26]. Specifically, conjugate gradient (CG) or molecular dynamics (MD) is implemented after each small compression (density increase) to find the nearest local energy minimum in the potential energy landscape (PEL). Then the system jams if the energy maintains finite. Using this method, O'Hern et al. found that point J, the ideal marginal jammed state in infinite system, coincides with RCPs, whose packing fractions are about 0.64 for monodisperse spheres and 0.84 for 50:50 binary disks with a size ratio of 1.4. Moreover, they clarified that distinct jammed configurations are not equiprobable upon those random initializations in small disk systems [26]. This argument shed some lights on the statistical approaches to understand the jammed systems and several recent studies have concentrated on this [5,27–29]. In brief, random gas-like configurations should jam at a unique density ϕ_J, as system size goes to infinity, provided they are compressed to corresponding inherent jammed states in PEL via aforementioned algorithms. Crucially, any barrier crossing behaviors can disturb the location of jamming onset, which may show a misleading density distribution. Recently, it was reported that jamming transition may occur at higher densities than usual ones for dense fluids [30–32]. Thus, for a system with infinite size, ϕ_J can only be obtained under two conditions: a truly random initial configuration and no barrier crossing in the PEL.

The arguments above can be directly extended to the cases of nonspherical particles. However, two major issues emerge due to the additional rotational degrees of freedom. Firstly, the uniqueness of ϕ_J can be easily disturbed for nonspherical particles due to their complex shapes. This effect should explain why many simulations and experiments provide controversial results about the critical states of nonspherical particles, e.g. tetrahedra and cubes, [23,24,33,34] although its physical foundation is not very clear now. Secondly, it is very computationally expensive to perform an accurate soft particle protocol, such as CG, to generate nonspherical packings at ϕ_J. The relationship between ϕ_J and the shape parameters is a main concern for nonspherical granular systems [2,3,21,35]. Then, certain approximated method can be useful at the cost of precision if one is more interested in some macroscopic properties rather than precise local structures in packings. This is exactly the starting point of this research.

Considering the aforementioned quasi-static compression protocol, we can always distinguish the obtained unjammed and jammed packings near ϕ_J via a preset energy threshold within any precision we want, regardless of the computational expense [26]. Then, the iteration step number in CG or time in MD will diverge approaching jamming for infinite system, which reflects the physical nature at this critical state. In glass scenarios, data fitting functions, namely Vogel–Fulcher–Tammann and so on, are applied to handle with this kind of divergence [36,37]. Different from that, we can also investigate over-jammed packings in soft model to approach ϕ_J from another side. Actually, the condition of constant densities can avoid possible dynamic effects of compression rate. Consequently, systems with densities well below or above ϕ_J will end up soon with no energy or steady finite energy respectively, while those near ϕ_J will keep decreasing their energy at an infinitesimal rate. This density controlled phenomenon should simply depict the jamming transition and it is a sufficient approximated method to determine the critical densities.

In this work, we study the jamming transition of a large variety of frictionless particles, including spheres, spherocylinders, ellipsoids, and spheropolyhedra. A simple geometric optimization method, the relaxation algorithm, [25,38–40] is used to investigate the system evolutions initialized randomly. By tracing the system overlap ratio over the iteration step number at different packing densities, we find a clear power-law scaling, which coincides with the jamming transition density. A data fitting function [41,42] is applied to obtain the characteristic time scale which diverges at the jamming transition. Compared with conventional jammed packing algorithms of soft particles, simulations at different densities are carried out simultaneously and then the transition density ϕ_J can be captured directly via the distribution of the obtained time scale. However, more elaborate techniques are still required if one concerns about careful structural analysis on packings at jamming onset, which can be accomplished by typical jammed packing algorithms. Thus, here we do not focus on the structural particularity at ϕ_J. The results of the jamming transition densities for various particle shapes agree well with several existing works, and provide some new insights into the shape effects on the jamming transition. Besides, we investigate the plastic behaviors of over-jammed packings for several particles under a compression–expansion procedure, which simply verifies their relative robustness at jamming.

2. Model and algorithm

In this work, we investigate the jamming transition of frictionless spherical and non-spherical particles, namely, sphere, spherocylinders, ellipsoids and spheropolyhedra (see Fig. 1). Several previous researches have provided results on the ϕ_J for ellipsoids, spherocylinders and several ideal polyhedra using different methods for both hard and soft particle models [23–25,43,44]. So, criticality at ϕ_J from both sides can further validate these results.

We apply a geometric optimization method, the relaxation algorithm, to perform the simulations for various particles as shown in Fig. 1. Similar to the typical soft particle method, overlap detection is performed for each pair of contacting