Universality of jamming of nonspherical particles

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Amorphous packings of nonspherical particles such as ellipsoids and spherocylinders are known to be hypostatic: the number of mechanical contacts between particles is smaller than the number of degrees of freedom, thus violating Maxwell’s mechanical stability criterion. In this work, we propose a general theory of hypostatic amorphous packings and the associated jamming transition. First, we show that many systems fall into a same universality class. As an example, we explicitly map ellipsoids into a system of “breathing” particles. We show by using a marginal stability argument that in both cases jammed packings are hypostatic and that the critical exponents related to the contact number and the vibrational density of states are the same. Furthermore, we introduce a generalized perceptron model which can be solved analytically by the replica method. The analytical solution predicts critical exponents in the same hypostatic jamming universality class. Our analysis further reveals that the force and gap distributions of hypostatic jamming do not show power-law behavior, in marked contrast to the isostatic jamming of spherical particles. Finally, we confirm our theoretical predictions by numerical simulations.

However, a system of spherical particles is an idealized model and, in reality, constituent particles are, in general, nonspherical. In this case, one should specify the direction of each particle in addition to the particle position. The effects of those extra degrees of freedom have been investigated in detail in the case of ellipsoids (2, 3, 9–32). Notably, the contact number at the jamming point continuously increases from the isostatic value of spheres, as $\zeta J = 2d - 41/2$, where $\Delta$ denotes the deviation from the perfectly spherical shape. The system is thus hypostatic: The contact number is lower than what is expected by the naïve Maxwell’s stability condition, which would predict $\zeta J = 2(d + d_{\text{ex}})$ where $d_{\text{ex}}$ is the number of rotational degrees of freedom per particle (9, 28, 29). As a consequence of hypostaticity, $D(\omega)$ has anomalous zero modes at $\zeta J$, which are referred to as “quartic modes” because they are stabilized by quartic terms of the potential energy (29–32). Hypostatic packings are also obtained for spherocylinders (33–37), superballs (38), superellipsoids (39), other convex-shaped particles (40), and even deformable polygons (41). Compared with spherical particles, the theoretical understanding of the jamming transition of nonspherical particles is still in its infancy (29, 42). In particular, the physical mechanism that induces a scaling behavior such as $\zeta J = 2d - 41/2$ is unclear.

In this work, we propose a theoretical framework to describe the universality class of hypostatic jamming. As a first example of universality, we map ellipsoids into a model of “breathing” spherical particles (BP), recently introduced in ref. 43. Based on the mapping, we show that the two models indeed have the same critical exponents by using a marginal stability argument. Next, we propose a generalization of the random perceptron model that mimics the BP and can be solved analytically using the replica method. We confirm that this model is in the same universality class of ellipsoids, BP, and other nonspherical particles that

Significance

The jamming transition is a key property of granular materials, including sand and dense suspensions. In the generic situation of nonspherical particles, its scaling properties are not completely understood. Previous empirical and theoretical work in ellipsoids and spherocylinders indicates that both structural and vibrational properties are fundamentally affected by shape. Here we explain these observations using a combination of marginal stability arguments and the replica method. We unravel a universality class for particles with internal degrees of freedom and derive how the structure of packings and their vibrations scale as the particles evolve toward spheres.

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display hypostatic jamming. This analysis further predicts the scaling behavior of $g(h)$ and $P(f)$ near the jamming point. Interestingly, we find that these functions do not show a power-law behavior even at the jamming point, in marked contrast to the jamming of spherical particles. Also the simplicity of the model allows us to derive an analytical expression of the density of states $D(\omega)$, which exhibits the very same scaling behavior as that of ellipsoids and BP. Finally, we confirm our predictions by numerical simulations of the BP model.

**BP Model**

The BP model (43) was originally introduced to understand the physics of the swap Monte Carlo algorithm (44), but here we focus on its relation with the jamming of ellipsoids. The model consists of $N$ spherical particles with positions $x_i$ in $d$ dimensions and radius $R_i \geq 0$, interacting via the potential energy

$$V_N(\{x\}, \{R\}) = U_N(\{x\}, \{R\}) + \mu_N(\{R\}),$$

where, defining $\theta(x)$ as the Heaviside theta function,

$$U_N = \sum_{i<j} k \frac{h^2}{2} \theta(-h_{ij}), \quad h_{ij} = |x_i - x_j| - R_i - R_j,$$

is the standard harmonic repulsive interaction potential of spherical particles such as bubbles and colloids (5), and the distribution of $R_i$, which can fluctuate around a reference value $R_0^i$, is controlled by the chemical potential term

$$\mu_N = \frac{k_R}{2} \sum_i (R_i - R_0^i)^2 (\frac{R_0^i}{R_i})^2.$$

Here, $k_R$ is determined by imposing that the dimensionless SD $\Delta \sim \sqrt{\sum_i (R_i - R_0^i)^2/N(R_0^i)^2}$ is constant, with $R_0 = N^{-1} \sum_i R_0^i$. Note that $\Delta = 0$ (corresponding to $k_R = \infty$) gives back the usual spherical particles (5) and that the full distribution of radii, $P(R)$, can generically change even if $\Delta$ is kept fixed. Upon approaching jamming, where the adimensionnal pressure $p$ (in units of $k_B T R_0^{-2}$) vanishes, it is found that $k_R = p/\Delta$ and $P(R)$ remains constant (43).

Because the BP model has $Nd$ translational degrees of freedom and $N$ radial degrees of freedom, the naive Maxwell stability condition requires $s \geq 2(d+1)$ in the thermodynamic limit (19, 45). However, a marginal stability argument and numerical simulations prove that the contact number at the jamming point $z_f$ increases continuously as $z_f \sim 2d \propto \Delta^{1/2}$ (43) and the system is hypostatic for sufficiently small $\Delta$; i.e., the number of constraints is smaller than that required by Maxwell’s stability condition. This is very similar to ellipsoids and motivates us to conjecture that the two models could belong to the same universality class. In the following, we show that this expectation is indeed true: Hypostatic packings of the BP and ellipsoids are stabilized by a common mechanism and have the same critical exponents.

**Mapping from Ellipsoids to BP**

We now construct a mapping from a system of ellipsoids to the spherical BP model introduced above. Ellipsoids are described by their position $x_i$ and by unit vectors $u_i$ along their principal axis, and for concreteness we model them by the Gay–Berne potential (31, 46)

$$V_N(\{x\}, \{u\}) = \sum_{i<j} v(h_{ij}), \quad v(h) = k \frac{h^2}{2} \theta(-h),$$

where the gap function is defined as

$$h_{ij} = |x_i - x_j| - \sigma_{ij}, \quad \sigma_{ij} = \frac{1}{\sqrt{1 + \frac{1}{\epsilon} \left( \frac{(u_i \cdot u_j + x_i \cdot x_j)^2}{1 - \epsilon} \right)^2}},$$

Here, $h_{ij} = r_{ij}/\sigma_0 - 1$ and $\Delta^2 w_{ij}$ denotes the $O(\Delta^2)$ term that we do not need to write explicitly. Substituting this in Eq. 4 and keeping terms up to $\Delta^2$, we obtain $V_N \approx U_N + \mu_N$, where

$$U_N = \sum_{i<j} v(h_{ij}) + \Delta^2 w_{ij}, \quad \mu_N = \frac{1}{2} \sum_i (\Delta u_i) \cdot \kappa_i \cdot (\Delta u_i).$$

The stiffness matrix is $k_s = -\Delta^{-1} \sum_{ij} v'(h_{ij}) \hat{r}_{ij} \hat{r}_{ij}$, where $a, b = 1, \ldots, d$. Note that near the jamming point, $k_s$ behaves as $k_s \sim (h/\Delta) \sim p/\Delta$, which is the same scaling of the stiffness $k_R$ of the BP model, Eq. 3. Hence, if we identify $\Delta u_i$ with $R_i$, in the vicinity of jamming the potential for ellipsoids can be analyzed essentially in the same way as in the BP model (43), as we discuss next.

**Marginal Stability**

The distinctive feature of both BP and ellipsoids is that the total potential, and thus the Hessian matrix, can be split into two parts: one having finite stiffness and the second one having vanishing stiffness $p/\Delta$ by dimensional arguments. The zero modes of the first term are stabilized by the second one, as recognized in refs. 29 and 32. We now provide additional insight on this structure by generalizing a marginal stability argument discussed for the BP in ref. 43. At jamming, $p = 0$ and $V_N = U_N$ because $\mu_N \propto p$. The $N_0 \equiv Nz/2$ constraints coming from $U_N$, one per mechanical contact, stabilize the same number of vibrational modes. Because the system is hypostatic, there remain $N_0 \equiv N(d + d_{\infty}) - N - 2z = N(d_{\infty} - z_{\infty})/2$ zero-frequency modes, where $z_{\infty} = z - 2d$ and $d_{\infty}$ is the number of extra degrees of freedom per particle; i.e., $d_{\infty} = 1$ for the BP and $d_{\infty} = d - 1$ for ellipsoids. Above jamming, where $p > 0$, the $N_0$ zero modes are stabilized by the “soft” constraint coming from $\mu_N$ whose characteristic stiffness is $k_s \sim (h/\Delta) \ll k$, where $k$ is the stiffness associated to $U_N$. Hence, the energy scale of these modes remains well separated from that of the $N_0$ other modes, and we can restrict to the $N_0$-dimensional subspace of the soft modes. In this space, we have $N_0^0 = (N - z_{\infty}/2)$ degrees of freedom, and $\mu_N$ provides $N_0^a$ constraints; hence the number of degrees of freedom is $N_{\infty} - z_{\infty}/2$ less than the number of constraints. When $z_{\infty} \ll 1$, a variational argument developed in refs. 17 and 47 describes the low-frequency spectrum. It shows that the soft modes are shifted above a characteristic frequency $\omega_{\infty}^2 \sim k_{b} z_{\infty}^2 \sim k_{b} \Delta^2(p/\Delta)$, which is reduced by $\sim -p$ by the so-called prestress terms, resulting in $\omega_{\infty}^2 = c_1 \Delta^{-1} p b d z^2 - c_2 p$, where $b$ and $c_1$ are constants.
where \( c_1 \) and \( c_2 \) are unknown constants. Assuming that the system is marginally stable, \( \omega_*(p) = 0 \), results in (43)

\[ \delta z \sim \Delta^{1/2}. \]  

This explains the universal square-root singularity of the contact number \( z_j \) observed in ellipsoids, BP, and several other models (9, 29, 43), as illustrated in Fig. 1. Eq. 8 holds when \( p \ll \Delta \) because in the argument we assumed to be close to jamming \((p \sim 0)\) at fixed \( \Delta \). On the contrary, when \( \Delta \sim p \), the contact number should have the same scaling of spherical particles:

\[ \delta z \sim p^{1/2}. \]  

Eqs. 8 and 9 imply that \( p \) and \( \Delta \) have the same scaling dimension and the following scaling holds:

\[ \delta z = \Delta^\gamma f(p/\Delta). \]  

In the \( \Delta \to 0 \) limit, Eq. 10 reduces to Eq. 9, which requires \( \gamma = 1/2 \) and \( f(x) \to x^{1/2} \) for \( x \gg 1 \). In the \( p \to 0 \) limit, we should recover Eq. 8, which requires \( f(x) \to \text{const} \) for \( x \ll 1 \). For the BP, Eq. 10 is confirmed by numerical simulations (43). Assuming that \( f(x) \) is a regular function around \( x \sim 0 \), one can expand it as \( f(x) = c_0 + c_1 x + \cdots \) and obtains

\[ z - z_j \sim \Delta^{-1/2} p, \]  

where \( z_j = 2d + c_0 \Delta^{1/2} \). This is compatible with previous numerical results of ellipsoids, where \( z - z_j \sim \Delta^{-0.5\pm 0.1} p \) (48). We can also study the response to shear deformation, which mainly excites the zero modes (30). Applying the argument in ref. 18 to the zero modes and using Eq. 8, the shear modulus \( G \) behaves as \( G \sim \delta z k_B \sim \delta z k_B \sim p/\sqrt{\Delta}, \) in perfect agreement with the numerical result (30).

**Vibrational Spectrum**

The marginal stability argument suggests that \( N_0 \) soft vibrational modes can be found in the frequency range \( \omega^* \lesssim \omega \lesssim \sqrt{k_B} \), with \( \omega^* \sim 0 \) due to marginal stability and \( k_B \sim p/\Delta \), while the remaining \( N_3 \) modes have finite frequency at jamming. We now refine the argument to discuss in more detail the vibrational density of states \( D(\omega) \). It is convenient to define the \( N \times N \) Hessian matrix of the BP model, with \( N = N(d + d_x) \), as the second derivative of the interaction potential \( V(x) \) w.r.t. \( x \), and \( R_i/\Delta \) in such a way that it has a similar scaling to the one of ellipsoids, where \( R_i/\Delta \) is mapped onto the angular degrees of freedom \( u_i \).

Then, \( D(\omega) \) near jamming can be separated into the following three regions: (i) \( \omega_0 = \omega_0(d_x - \delta z/2) \) zero modes stabilized by \( \mu_S \). Their typical frequency is \( \omega^0_0 \sim \partial^2 \mu_S / \partial (\Delta^{-1} R_i^2)^2 \sim k_B \Delta^{2} \sim \Delta_p \). The remaining \( N_3 = N - N_0 = N_0/2 \) modes can be split into two bands: (ii) an intermediate band corresponding to the extra (rotational or radial) degrees of freedom \( N_1 = N_0 \delta z/2 \), with typical frequency \( \omega_1^0 \sim \partial^2 V / \partial (\Delta^{-2} R_i)^2 \sim \Delta^2 \), and (iii) the highest band corresponding to the \( N_2 = Nd \) translational degrees of freedom. For \( \Delta \ll 1 \), the additional degrees of freedom do not strongly affect these modes, and one can apply the standard variational argument of spherical particles (17, 47), which predicts that their typical frequency is \( \omega^0_2 \sim \delta z \sim \Delta \). The resulting \( D(\omega) \) differs significantly from that of isostatic packings of spherical particles, which displays a single translational band.

Numerical results for \( D(\omega) \) of ellipsoids from ref. 30 and of the BP from ref. 43 and analytical results for the perceptron model introduced below are reported in Fig. 2. Details about the simulations of the BP are explained in ref. 43; here we show data for \( N = 484 \) particles, averaged over at least 1,000 samples for each state point. As predicted by our theory, \( D(\omega) \) consists of three separated bands with characteristic peak frequencies \( \omega_{0,1,2} \). Their scaling with \( \Delta \), also reported in Fig. 2 at fixed \( \Omega \), follows the theoretical predictions \( \omega_{0,1,2} \propto 1/\sqrt{\Delta} \). For small \( \Delta \), we also find that \( \omega_2 \propto p/\sqrt{\Delta} \) for small \( p \), while \( \omega_{0,1} \) do not change much with \( p \), which is again consistent with the theory. Finally, in Fig. 3 we report the fraction \( f_i = N_i/N \) of modes in each band for the BP, which also follow the theoretical prediction as a function of \( \Delta \) and \( p \).

**Mean-Field Model**

The universality class of isostatic jamming is well understood: It can be described analytically by particles in \( d \to \infty \) (15) or, equivalently, by the perceptron model (24–26). Both models reproduce the critical exponents of isostatic jamming in all dimensions \( d \), leading to the conjecture that its lower critical dimension is \( d = 2 \) (49).

We now introduce a mean-field model which describes the universality class of hypostatic jamming in the BP, ellipsoids, and many other models of nonspherical particles. The model, which is a generalization of the perceptron, can be solved analytically and, as we show, the solution reproduces all of the critical exponents of hypostatic jamming. It consists of one tracer particle with coordinate \( x \) on the surface of the \( N \)-dimensional hypersphere of radius \( \sqrt{N} \) and \( M \) obstacles of coordinates \( \xi_i \) and “size” \( \sigma + R_i \). The interaction potential between the tracer particle and the obstacles is

\[ V_N = U_N + \mu_N, \ \mu_N = \sum_{i=1}^{M} v(h_i), \ \mu_B = k_B M \sum_{i=1}^{M} R_i^2, \]  

where \( v(h) = h^2 \theta(-h)/2 \) and the gap variable \( h_i \) is defined as

\[ h_i = x \cdot \xi_i - \sigma - R_i. \]  

The \( \xi_i \) are frozen variables, and each of their components follows independently a normal distribution of zero mean and unit
Fig. 2. Universality of the density of states. (Top) Density of states for ellipses, BP, and the perceptron. (Bottom) Evolution with $\Delta$ of the characteristic frequencies at $p = 10^{-4}$. Solid lines denote the theoretical predictions, $\omega_0 \propto \Delta^{1/2}$, $\omega_1 \propto \Delta$, and $\omega_2 \propto \Delta^{1/2}$, respectively. Data of ellipses are reproduced from ref. 32.

Because the model can be solved by the same procedure as that of the standard perceptron model, here we give just a brief sketch of our calculation. The free energy of the model at temperature $T = 1/\beta$ can be calculated by the replica method, $-\beta f = \lim_{n \to 0} \frac{1}{nN} \log Z_n$, where $Z = \int d^N x d^M \xi e^{-\beta V_x}$ and the overbar denotes the averaging over the quenched randomness $\xi$. Here we are interested in the athermal limit $T \to 0$. Using the saddle-point method, the free energy can be expressed as a function of the overlap $q_{ab} = \langle x^a \cdot x^b \rangle / N$, where $x^a$ and $x^b$ denote the positions of the tracer particles of the $a$th and $b$th replicas, respectively. In the $n \to 0$ limit, $q_{ab}$ is parameterized by a continuous variable $x \in [0, 1]$. $q_{ab} \to q(x)$. The function $q(x)$ plays the role of the order parameter and characterizes the hierarchical structure of the metastable states (50). We first calculate the phase diagram assuming a constant $q(x) = q$, which is the so-called replica symmetric (RS) ansatz that describes an energy landscape with a single minimum. The result for $\Delta = 0.1$ is shown in Fig. 4. The control parameters are the obstacle density $\alpha = M/N$ and size $\sigma$. If $\alpha$ is small, the tracer particle can easily find islands of configurations $x$ that satisfy all of the constraints $h_\mu > 0$: The total potential energy $U_N$ and the pressure vanish and the system is unjammed. The overlap $q < 1$ measures the typical distance between two zero-energy configurations. Upon increasing $\alpha$, $q$ increases and eventually reaches $q = 1$ at $\alpha_J$, which is the jamming transition point (Fig. 4). Naturally, due to the additional degrees of freedom when $\Delta > 0$, we have $\alpha_J(\Delta) > \alpha_J(0)$ for equal $\sigma$. For $\sigma > 0$, the RS ansatz is stable for all values of $\alpha$ and it describes the jamming transition. For $\sigma < 0$ instead, the jamming line is surrounded by a RSB region where the RS ansatz is unstable. The jamming transition should thus be described by the RSB ansatz where $q(x)$ is not constant, corresponding to a rough energy landscape. The qualitative behavior of the phase diagram is independent of $\Delta$; in

Fig. 3. Weights of the density of states. Shown is the fraction of modes $f_i = N_i / N$ in the three bands of $D(\omega)$ given in Fig. 2, plotted as functions of $p$ at fixed $\Delta = 10^{-1}$ (Left) and $\Delta$ at fixed $p = 10^{-4}$ (Right) for BP (with $d = 2$ and $d_{ex} = 1$). The theoretical predictions $f_0 = (1 - 4\xi) / 2$, $f_1 = 4\xi / 6$, and $f_2 = 2 / 3$ are plotted as solid lines, inferred from the measured $\delta z$. 

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with new critical exponents $\mu = \kappa/(4\kappa - 4) = 0.851$ and $\nu = \mu - 1/2$ and a universal scaling function $p_0(x)$. The scaling analysis also leads to $z_J - 1 \sim \Delta^{1/2}$ and $c_\Delta \sim \Delta^{-1/2}$, consistent with the marginal stability argument, Eqs. 8 and 11.

The simplicity of the model allows us to derive the analytical form of the density of states $D(\omega)$. As before, we define the Hessian matrix as the second derivatives of the interaction potential $V_N$, Eq. 12, w.r.t. $x_i$ and $R_i/\Delta$. Using the Edwards–Jones formula for the eigenvalue density $\rho(\lambda)$ (51, 52), the density of states $D(\omega) = 2\pi\rho(\omega^2)$ can be expressed analytically in closed form as a function of $z$, $k_0$, and $p$.

These quantities should be obtained by solving numerically the full RSB equations but for simplicity, because here we are interested only in the scaling properties of $D(\omega)$, to obtain Fig. 2 we used arbitrary functions $z$, $k_0$, and $p$ which are compatible with the analytical scaling derived from the full RSB equation. We find that $D(\omega)$ displays three separate bands (Fig. 2). As in the standard perceptron (24), marginal stability in the full RSB phase implies that the lowest band starts from $\omega = 0$ and for small $\omega$, $D(\omega) \sim \omega^2$.

The lowest band terminates at $\omega_0 \sim \Delta^{1/2}p^{1/2}$ near which $D(\omega)$ exhibits a sharp peak. At $\omega_0 \sim \Delta$ a delta peak is found, while the highest band starts from $\omega_0 \sim \Delta^{1/2}$. The qualitative behavior of $D(\omega)$ and the scaling of $\omega_0$, $\omega_1$, and $\omega_2$ are the same as those of all of the models displaying hypostatic jamming, such as ellipsoids (31, 32) and BP (43). This confirms that the generalized perceptron can reproduce analytically all of the critical properties of the hypostatic jamming transition.

As a final check of universality, we test the prediction for the $\Delta$ dependence of the gap distribution function $g(h)$ at the jamming point, Eq. 14. In Fig. 5, we show numerical results (obtained as in ref. 43) for $g(h)$ of the BP model at $p = 10^{-6}$, a value small enough to observe the critical behavior. Here, as usual for particle systems, $g(h)$ is normalized by $g(h) \rightarrow 1$ for large $h$. When $\Delta = 0$, $g(h)$ exhibits a power-law divergence, $g(h) \sim h^{-\gamma}$, where $\gamma = 0.413$, consistent with previous numerical observation (6, 14, 15). For finite $\Delta$, on the contrary, the divergence of $g(h)$ is cut off (Fig. 5), consistent with the theoretical prediction of Eq. 14.

**Conclusions**

Using a marginal stability argument, we derived the scaling behavior of the contact number $z$ and the density of states $D(\omega)$ of ellipsoids and breathing particles. Our theory predicts that the scaling behaviors of the two models are identical, which we confirmed numerically. Many other models of nonspHERical particles display the same jamming criticality (40), which defines another universality class of hypostatic jamming. We
introduced an analytically solvable model which allows us to derive analytically the critical exponents associated to this universality class.

One of the most surprising outputs of our theory is the universality of the density of states $D(\omega)$ (Fig. 2). This might be relevant for some colloidal experiments where the constituents are quite spherical (53) in which the vibrational modes could be experimentally extracted from the fluctuations of positions (54, 55).

Another relevant question is how nonspherical particles would flow under shear (30). The divergence of the viscosity at jamming is related to the low eigenvalues of $D(\omega)$ (56), which suggests that the shear flow of nonspherical particles should be quite different from that of spherical particles, in agreement with recent experiments (57).

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