Jamming as a critical phenomenon: a field theory of zero-temperature grain packings

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A field theory of frictionless grain packings in two dimensions is shown to exhibit a zero-temperature critical point at a non-zero value of the packing fraction. The zero-temperature constraint of force-balance plays a crucial role in determining the nature of the transition. Two order parameters, $\langle z \rangle$, the deviation of the average number of contacts from the isostatic value and, $\langle \phi \rangle$, the average magnitude of the force per contact, characterize the transition from the jammed (high packing fraction) to the unjammed (low packing fraction state). The critical point has a mixed character with the order parameters showing a jump discontinuity but with fluctuations of the contact force diverging. At the critical point, the distribution of $\phi$ shows the characteristic plateau observed in static granular piles. The theory makes falsifiable predictions about the spatial fluctuations of the contact forces. Implications for finite temperature dynamics and generalizations to frictional packings and higher dimensions are discussed.

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Introduction In a remarkably diverse range of systems, the transition from a flowing, liquid state to a jammed, solid state is heralded by a dramatic slowing down of relaxations. Does an equilibrium critical point underlie this glassy dynamics? The debate surrounding this question has been spurred by the absence of any obvious static signature accompanying the rapid increase of time scales. Purely dynamical scenarios have been proposed to explain time-scale divergences with no accompanying static divergences. For thermal systems, a different perspective has been offered within the framework of an avoided critical point and a scaling theory based on the existence of a zero-temperature critical point. In a more recent development, it has been suggested that the mechanism of jamming in both thermal and athermal systems is controlled by a zero-temperature critical point (J-point).

Experiments on weakly sheared granular media indicate that at a critical packing fraction there is a transition accompanied by slow dynamics, vanishing of mean stress, increasing stress fluctuations and a change in the distribution of contact forces. Simulations indicate a critical point occurring at zero temperature and a packing fraction close to the random close packing value. A theory based on this observation predicts a diverging length scale associated with the mechanical stability of the network. In a different theoretical approach, an analogy has been drawn between the jamming transition and k-core percolation.

In the present work, it is shown that a statistical field theory of two-dimensional, zero-temperature, frictionless grain packings exhibits a critical point. This point separates a disordered phase from an “ordered” one characterized by two order parameters: (i) the magnitude of the force per contact, $\langle \phi \rangle$, and (ii) $\langle z \rangle$, the deviation of the contact number per grain from its isostatic value. At the critical point, the fluctuations around $\langle \phi \rangle$ diverge but those around $\langle z \rangle$ go to zero. An analytic prediction for $P(F)$, the distribution of contact forces, is in excellent agreement with experiments, and the theory makes falsifiable predictions regarding the spatial correlations of the forces.

Statistical Ensemble In granular matter, which is athermal, a natural control parameter is the packing fraction. For short-range repulsive potentials, the corresponding statistical ensemble is one with a fixed average pressure. The probability $P\{ \{ r_i \} \}$ of a grain packing with the set of positions $\{ r_i \}$ can be obtained by using the maximum entropy principle, which also forms the basis of the Edwards ensemble of granular packings. Maximizing the entropy, $S[P] = -\sum_i P\{ \{ r_i \} \} \ln P\{ \{ r_i \} \}$ subject to the constraint of fixed average pressure leads to:

$$P\{ \{ r_i \} \} = (1/Z) \exp(\alpha p(\{ r_i \})) \quad (1)$$

where $p(\{ r_i \}) = (1/V) \sum_{ij} r_{ij} \partial U/\partial r_{ij}$ is the pressure of the configuration $\{ r_i \}$ ($U$ is the interaction potential). The “canonical” partition function, $Z(\alpha) = \sum_{\{ r_i \} \{ P(\{ r_i \} \) \}}$ is the generating function of all statistical averages. The Lagrange multiplier $\alpha$ plays the role of inverse temperature: $\alpha = -\partial S/\partial p$ and the prime on the summation restricts it to grain configurations satisfying the equations of mechanical equilibrium for frictionless packings in $d$ dimensions:

$$dN \text{ eqs: } \sum_j F_{ij} \frac{r_{ij}}{r_{ij}} = 0 \quad (2)$$

$$\langle z \rangle N/2 \text{ eqs: } F_{ij} = f(r_{ij}) \quad (3)$$

Here $\langle z \rangle$ is the average number of contacts per grain, $F_{ij}$ is the magnitude of the contact force between grains.
FIG. 1: Illustration of height field. The dashed lines are contact forces and the heights associated with the loops are represented by the arrows encircling a loop

The positions $i$ and $j$, and $f(r_{ij})$ is the function specifying the inter-grain force law. At the isostatic point, $<z> = z_{iso} = 2d$, the number of equations in Eq. 2 is exactly equal to the number of unknown forces, $F_{ij}$ and, therefore, the forces are uniquely determined by these equations. The positions $\{r_i\}$ can then be obtained by inverting Eq. 3. For $<z> > z_{iso}$, Eqs. 2 and 3 are coupled and the coupling can be parametrized by $\epsilon$ which encodes how sensitive the contact forces are to changes in the grain $\epsilon < z_{iso}$, the contact forces through: $\mathbf{F}_{ij} = \mathbf{h}_{ij} - \mathbf{h}_p$ where $j'$ and $i'$ are the voids bracketing the contact $ij$ (cf. Fig. 1).

Since the $\mathbf{F}_{ij}$’s around a grain sum to zero, the mapping of forces to heights is one to one, up to an arbitrary choice of a single height. For frictionless grains, the requirement of $\mathbf{F}_{ij}$ being parallel to $\mathbf{r}_{ij}$ leads to restrictions on the heights. In developing the field theory, the heights are coarse grained over a mesoscopic region with a length scale much larger than the grain radius but smaller than a typical length scale over which the height fields vary to define a continuous height field. It can be shown that the constraint on the coarse-grained field resulting from the frictionless property is that the heights be divergence free and, in 2d, this implies that the height field can be written in terms of a scalar potential $\psi$: $h_x = \partial_x \psi : h_y = -\partial_y \psi$. A similar approach lead to the definition of a potential for frictional grain-packings.

The coarse-grained field $\psi$ carries with it a weight $\Omega[\psi]$ which counts the number of microscopic configurations giving rise to the same $\psi$ field. Arguments similar to those employed in height-maps of loop models, lead to $\Omega[\psi] \sim e^{-(1/2)\int d^2r \nabla^2 \psi^2}$. The basic reasoning is that configurations which are completely flat, i.e. $\nabla^2 \psi = 0$, have the largest number of loops (dashed in Fig. 1) along which the contact forces can be shuffled without violating the force-balance constraint and, therefore, are favored entropically.

At the isostatic point, $z = z_{iso}$, $p = \nabla^2 \psi$. For packings close to the isostatic one, an expansion in $z - z_{iso}$ leads to

$$p(r) = \nabla^2 \psi + (z - z_{iso}) \frac{\Delta p}{\Delta z} \bigg|_{z_{iso}}$$

$$= \nabla^2 \psi + (z - z_{iso}) \frac{\Delta^2 \psi}{\Delta z^2} \bigg|_{z_{iso}} = z \frac{\Delta^2 \psi}{\Delta z^2}.$$  (6)

The second set of equations follow by noting that the extra pressure, $\frac{\Delta^2 \psi}{\Delta z^2}$, due to the introduction of an additional contact at the isostatic point is the pressure at this packing divided by the number of contacts. Just as the mapping from $F_{ij} \rightarrow \psi$, the mapping from $r_i$ to the coarse-grained pressure, $p(r)$, involves the calculation of a weight $\omega[p]$. It can be argued that $\omega[p] \sim \exp(-K(\nabla p)^2)$ by picturing the packing of $N$ grains in a volume $V$. Entropically, it is favorable to have the grains occupy as much of the volume as possible, leading to small spatial variations of the packing density and
Large pressure gradients occur in the entropically unfavorable packings where there are large variations in the packing density.

With these weights, the partition function is:

\[
Z = \sum_{\{z\}, \{\psi\}} \Omega(\psi) \omega[p] \left\{ e^{\alpha z} \right\} \left[ e^{-\epsilon/2} \right] e^{-\epsilon/2} \left\{ d^4r(r) \right\}^2
\]

\[
= \sum_{\{z\}, \{\psi\}} e^{-H[\psi, z]}
\]

\[
H = \sum_q \left[ \left\{ \frac{1}{2} \right\} |\phi_q|^2 - \alpha (z_{iso} \delta_q + z - q) \phi_q \right] + V^{-1} \sum_{q_1, q_2, q_3, q_4} \left[ \frac{\epsilon}{2} - \frac{K}{2} (q_1 + q_3) \cdot (q_2 + q_4) \right]
\]

\[
[z_{iso}, z_2, \phi_1, \phi_2, \delta_1, \ldots, \delta_4]
\]

Here, \( \phi = \nabla^2 \psi \) represents the magnitude of the force per contact (cf Eq. 4), and the field \( z \) has been redefined to \( z - z_{iso} \) which is restricted to the set of integers. The parameters \( \alpha, \epsilon \) and \( K \) have been scaled to absorb resulting factors of \( z_{iso} \).

**Critical Point** The Hamiltonian \( H \) reflects the competition between \( \Omega[\psi] \) favoring \( \phi = 0 \) and the “field” \( \alpha \) favoring non zero \( \phi \). It provides a model for studying the response functions of grain packings with small but finite \( \epsilon \). We assume that the integer restriction on \( z \) can be ignored as long as \( \epsilon \neq 0 \).

In investigating whether or not there is a finite-\( \alpha \) phase transition involving the vanishing of one or more order parameters, the fields in the Hamiltonian in Eq. 6 are expanded around their average values: \( \phi_q = <\phi_q> + \zeta_q \), \( z_q = <z_q> + \eta_q \) and the hamiltonian written as \( H = H_0(<\phi_q>, <z_q>) + H_1(<\phi_q>, <z_q>; \zeta_q, \eta_q) \). The order parameters \( <\phi_q> \) and \( <z_q> \) are obtained by minimizing the effective potential, \( \Gamma(<\phi_q>, <z_q>) = H_0(<\phi_q>, <z_q>) - \ln \int \Omega(\psi) \left\{ d\zeta_q d\eta_q e^{-H_1} \right\} \). The simplest, non-trivial approximation, is obtained by calculating the fluctuations, \( <|q|^2> \) and \( <|q|^2> \), at the loop level, replacing all 4-point averages by 2-point averages [21], and assuming spatially uniform order parameters: \( \phi = 0 \), \( z = 0 \). To leading order in \( \epsilon \):

\[
<|q|^2> = 1 + \epsilon <z>^2 - 1/ <\phi>^2 + K <z> <\phi>^2
\]

\[
<|q|^2> = \epsilon <\phi>^2 + K <\phi>^2 <z>^2
\]

Incorporating these results in the effective potential and minimizing with respect to the order parameters leads to:

\[
<\phi> - \alpha (z_{iso} + <z>) + \epsilon <z>^2 <\phi> + \frac{1}{<\phi>} = 0
\]

\[
\epsilon (<\phi>^2 + \frac{1}{1 - 1/ <\phi>^2}) <z> - \alpha <\phi> = 0
\]

Solving these equations near \( \alpha_c = 2/z_{iso} \), the order parameters behave as:

\[
<\phi> = (\alpha/\alpha_c)(1 + (1 - \alpha_c/\alpha)^{1/2})
\]

\[
<z> = (\alpha/\alpha_c)(1 - \alpha_c/\alpha)^{1/2}
\]

For \( \alpha \geq \alpha_c \), there is an ordered phase characterized by two order parameters. For \( \alpha < \alpha_c \), \( \Gamma(<\phi>, <z>) \) ceases to have any local minima or maxima (cf Fig. 2) and \( <\phi> \) jumps discontinuously to 0: the physical limit of its allowed values. From Eqs. 8 and 10 as \( \alpha \to \alpha_c, \phi \to 1 \) and the \( q = 0 \) force fluctuations diverge: \( <\phi^2> - <\phi>^2 \sim (1 - \alpha_c/\alpha)^{-1/2} \). This type of transition is indicative of the end of a line of metastable equilibrium similar to spinodal critical points. Unlike spinodals, however, the transition is accompanied by the disappearance of any local minimum; a phenomenon observed in models with rigid constraints such as certain dimer models [21]. The fluctuations of \( z \) vanish as \( <z^2> - <z>^2 \sim (1 - \alpha_c/\alpha)^{1/2} \).

The structure factor of the magnitude of the contact forces (the \( \phi \) field), \( S(q) \equiv <|q|^2> \), provides detailed, measurable information about the spatial fluctuations of the contact force. Eq. 8 predicts

\[
S(q) = \frac{1}{\xi/a(\epsilon, K)} + q^2 \xi^2
\]

where \( \xi \approx (1 - 1/ <\phi>^2) \approx (1 - \alpha_c/\alpha^2)/\langle z > \) and \( a(\epsilon, K) \) is a characteristic length scale of the model. The length scale \( \xi \) vanishes at the critical point and \( S(q = 0) \) diverges as \( 1/\xi \). There is another length scale related to the width of the structure factor peak: \( l^{-1} \equiv q_0 \) where \( q_0 = 1/\sqrt{2 \xi} \). The width diverges as \( (1 - \alpha_c^2/\alpha^2)^{-1/4} \). The appearance of these two length scales, and the specific form of \( S(q) \), are predictions of the theory that should be testable in experiments and simulations. The length scales, \( l \) and \( \xi \), are associated with correlations of contact forces and their vanishing implies that the length scale over which the packing behaves as an elastic solid is going to zero or, equivalently, the length scale over which the packing is floppy is diverging. The two exponents, 1/2 and 1/4, associated with the divergence of these complementary length scales are reminiscent of the exponents discussed in theories and simulations of J-point [2, 17] and simulations [10, 17] have shown that changes in the distribution of \( P(F) \) are associated with transitions involving the vanishing of stress. In the field theory, \( <\phi> \) corresponds to \( F \) and the distribution, \( P(<\phi>) \approx e^{-\Gamma(<\phi>, <\phi>)} \). The critical regime has \( <z> \to 0 \) (cf Eq. 10) implying \( \Gamma(<\phi>, <\phi>) \approx (1 - \alpha_c/\alpha^2) \). The term \( \ln <\phi> \) term results from integrating out the \( z \) field and embodies the physical effect of large contact number fluctuations for small contact forces. This term leads to a power-law decay \( P(<\phi>) \sim 1/ <\phi> \) near \( \phi = 0 \) and provides a qualitative explanation of the experimental data [3]. Fig. 2 clearly demonstrates that the approach to \( \alpha_c \) is accompanied by changes in the low-force regime of \( P(F) \) with a peak giving away to a plateau as the force fluctuations diverge. Since diverging force fluctuations imply vanishing
of the shear modulus \( \alpha - \alpha_c = 0.7, 0.5 \) and 0.025. The inset shows the \( <z>=0 \) cut of the potential, \( \Gamma(<\phi>,<z>) \) at different \( \alpha \) with \( \alpha \rightarrow \alpha_c \) from bottom to top.

Conclusions A field theory, founded on general properties of \( T = 0 \) packings of frictionless grains in two-dimensions, exhibits a critical point separating a jammed, “ordered” phase with finite yield stress at large packing fractions \( (\alpha > \alpha_c) \) from an unjammed phase where the order parameters vanish. A hallmark of the transition is a change in the distribution of contact forces reflecting diverging force fluctuations. Two length scales, associated with the spatial fluctuations of the contact forces, are predicted to go to zero at the critical point and should be detectable in experimental measurements of the structure factor of contact forces.

If the zero-temperature critical point controls the low temperature and weakly-driven behavior, then glassy dynamics follows from general scaling arguments. At finite temperatures, the force-balance constraint is violated and the height-field has defects. The interactions between these defects determine the stability of the zero-temperature critical point and, therefore, it will be crucial to understand these interactions. The extension of the theory to frictional packings is within reach since the loop-force formalism exists. Although the similarities between two and three dimensions, observed in simulations, suggest that an extension to higher dimensions is possible, this remains an open question.

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10. The simulations of J-point (Ref 5) were performed in an ensemble where the pressure is controlled, a “micro-canonical” ensemble.
17. S. Henkes and Bulbul Chakraborty, unpublished