Amorphous solids increase their stress as a function of an applied strain until a mechanical yield point whereupon the stress cannot increase anymore, afterwards exhibiting a steady state with a constant mean stress. In stress controlled experiments the system simply breaks when pushed beyond this mean stress. The ubiquity of this phenomenon over a huge variety of amorphous solids calls for a generic theory that is free of microscopic details. Here we offer such a theory: the mechanical yield is a thermodynamic phase transition, where yield occurs as a spinodal phenomenon. At the spinodal point there exists a divergent correlation length which is associated with the system-spanning instabilities (known also as shear bands) which are typical to the mechanical yield. The theory, the order parameter used and the correlation functions which exhibit the divergent correlation length are universal in nature and can be applied to any amorphous solids that undergoes mechanical yield.

A solid, be it crystalline or amorphous, is operatively defined as any material capable to respond elastically to an externally applied shear deformation (1). However, any solid material, when subjected to a large enough shear-strain, finally undergoes a mechanical yield. Here we focus on the mechanical yield of amorphous materials such as molecular and colloidal glasses, foams, and granular matter. The phenomenology exhibited by the yielding point within this vast class of materials, as reported in countless strain-controlled simulations (2–8) and experiments (9–11) shows a remarkable degree of universality despite the highly varied nature of the model systems involved. Among these universal features is the presence, at the onset of flow at yielding, of system spanning excitations referred to as shear-bands (12, 13), wherein the shear strongly localizes, leaving the rest of the material unperturbed. This phenomenon is of capital importance for engineering applications as it is responsible for the brittleness typical of glassy materials, in particular metallic glasses (14), whose potential for practical use is stymied by their tendency to shear-band and fracture (13, 15, 16).

In ametal amorphous solids the phenomenon has universal features. For strains \( \gamma \) smaller than some critical value denoted as \( \gamma_c \), the stress in the material grows on the average when the strain is increased. After yield the stress cannot grow on the average, no matter how much the strain is increased. The universality of the basic phenomenology of yielding begs a picture of its characteristics in terms of a universal theory, in the sense that such a theory should rely on a statistical-mechanical framework and be independent of details such as chemical composition and production process of the material. This need was addressed in a recent work (17), wherein building up from ideas first advanced in (18) there emerged a picture of mechanical yielding as a first-order phenomenon, i.e., as a discontinuous phase transition in a suitable overlap order parameter \( Q_{ab} \) (defined in Eq. (1) below) which jumps from a value of order 1 to a value of order zero as strain is increased above the yielding threshold \( \gamma_c \). The physical meaning of this observation is that before yielding the amorphous system was limited to a small patch in the configuration space, very far from any kind of ergodicity. The yielding transition is an opening of a much larger available configuration space, whereupon the system is ergodized subject to the constraint of constant mean stress. Within this framework, the yielding transition is essentially envisioned as a spinodal point (19) i.e. the point where the metastable, high \( Q_{ab} \), glassy phase of available configurations becomes unstable with respect to a new phase with low \( Q_{ab} \), associated with an ergodized system in the presence of disorder (20). A paradigmatic example of such a spinodal is the Mode Coupling crossover (12), characterized by dynamical slowing down and heterogeneities, whose behavior is characterized by a dynamical lengthscale which can be extracted from suitable multi-point correlators (12). According to our picture, this kind of critical behavior should also be found at the yielding transition, conditional that one is able to derive the expression of the right correlator to measure. This suggestion seems even more reasonable in light of a recent study (21) wherein the similarity of shear bands with dynamical heterogeneities has been pointed out; also, some oscillatory shear simulations seem to indicate that a slow-down of the dynamics on approaching yielding may indeed be present (22, 23). It is important to stress here that the reason that a spinodal

**Significance Statement**

The art of making structural, polymeric, and metallic glasses is rapidly developing with many applications. A limitation is that under increasing external strain all amorphous solids have a yield stress which, when exceeded, results in a plastic response leading to mechanical failure. Understanding this is crucial for assessing the risk of failure of glassy materials under loads. The universality of the mechanical yield requires a theory that is general enough to transcend the microscopic details of different glasses, which all show similar stress-strain curves with a yield point. We provide what appears to be the first general theory which is thermodynamic in nature, showing that the mechanical yield is a spinodal criticality in an appropriately constructed free energy landscape.

*GP, IP and CR designed research. IP, CR and MS performed research and analyzed data, and IP and CR wrote the paper.*

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point can be exposed and measured is that the glassy time scales and the athermal conditions stabilize the metastable system until the spinodal point is crossed and the system becomes unstable against constrained ergodization.

Within a generic statistical-mechanical-theory, formulated in terms of a suitable Gibbs free energy $G[\phi]$ (i.e., the free-energy for fixed order parameter $\phi$), stable phases are identified with its points of minimum in $\phi$, and phase transitions happen when the curvature of these minima goes to zero, inducing a critical behavior which manifests diverging susceptibilities-fluctuations, critical slowing down of the dynamics, and growing correlation lengths (24). At a spinodal point, for example, one such minimum becomes unstable and transforms into a saddle. In the case of the order parameter $Q_{ab}$ the general form of the free energy $s[Q_{ab}]$ had been already derived and studied (see (25) for a review) in the context of the theory of replicas originally developed for the study of spin-glasses, and its properties, at least at mean-field level, are well known (we refer to (18, 26) for the derivation of $s[Q_{ab}]$ in the specific case of mean-field hard spheres); the matrix of second derivatives (or, using a more field-theoretic terminology, the mass matrix) is not diagonal in the base of $Q_{ab}$, and after diagonalization is found to have only three distinct modes, or masses (25). Of these, the most relevant ones are the so-called replicon mode $\lambda_{R}$, which for example, zero to at the newly proposed Gardner transition (27), and the longitudinal mode $\lambda_{L}$ which is instead related to spinodal points (18, 19) such as our yielding transition. In the Supplementary Information to this paper we review briefly the background theory that is at the basis of the present approach.

In this paper, we build up from the results of (17) and, following the line of reasoning formulated above, we employ the expression of the correlation function relative to the longitudinal mode $\lambda_{L}$ as it can be derived from the replicated field theory (25) to reveal the critical features of the yielding transition. We measure this correlator in numerical simulation, and use it to expose the critical properties of the yielding correlation length encoded in this correlator. We show how the order parameter $Q_{ab}$ and its associated replicated field theory are thereby able to provide a unified and universal picture of the yielding transition in terms of a spinodal point in presence of disorder, with an associated criticality.

### The correlation functions

The relevant order parameter for the problem at hand is the overlap function $Q_{ab}$ which measures the distance between two configurations "a" and "b" of the same system. Denoting the position of the $i$th particle as $r_i^{a}$ in configuration "a" and $r_i^{b}$ in configuration "b" we define

$$Q_{ab} \equiv \frac{1}{N} \sum_{i=1}^{N} \theta(\ell - |r_i^{a} - r_i^{b}|) ,$$

where $\theta(x)$ is the Heaviside step function and $\ell$ is a constant length which is taken below to be 1/3 in Lennard-Jones units (see below for numerical details). Thus $Q_{ab} = 1$ for two identical configurations and $Q_{ab} = 0$ when the distance between the positions of all the particles $i$ in the two configurations exceed $\ell$. Based on the introductory discussion, we now derive an expression for the correlator associated with the longitudinal mode, from whence one can extract the correlation length associated with the onset of criticality at the yielding point, and define an associated susceptibility which will shoot up as the yielding point is approached. The first step is to "localize" the overlap function and define the $r$-dependent quantity

$$Q_{ab}(r) \equiv \sum_{i=1}^{N} \theta(\ell - |r_i^{a} - r_i^{b}|) \delta(r - r_i^{a}) .$$

Next, as mentioned above, the expression for the longitudinal correlator in terms of four-replica correlation functions can be found by diagonalization of the correlation matrix $G_{abcd}$, which is defined as the inverse of the mass matrix $M_{abcd}$ of the replicated field theory of the overlap order parameter $Q_{ab}$. The derivation is a matter of standard diagonalization algebra, so we shall not report it here and refer to the SI for the details. The expression, employed for example in (28, 29) in the case of a model with spins on a lattice, reads for athermal systems

$$G_L(r) = 2G_R(r) - \Gamma_2(r) ,$$

with the definitions

$$G_R(r) \equiv \langle Q_{ab}(r)Q_{ab}(0) \rangle - 2\langle Q_{ab}(r)Q_{ab}(0) \rangle ,$$

$$\Gamma_2(r) \equiv \langle Q_{ab}(r)Q_{ab}(0) \rangle - \langle Q_{ab}(r) \rangle \langle Q_{ab}(0) \rangle .$$

Here angular brackets denote a thermal average in the thermal case and an evaluation in an inherent state in the athermal case; an $[\cdot]$ indicates an average over different samples of the glass. The quantity $G_R(r)$ is the correlation function of the replicon mode (25) and $\Gamma_2(r)$ is just the garden-variety four-point correlator.

Using these definitions and taking Eq. (2) into account, the quantities we compute in numerical simulation, before taking the ensemble average, are (see the SI and Ref. (30)):

$$\Gamma_2(r) = \sum_{i \neq j} (u_{ij} - Q_{ab})(u_{ij} - Q_{ab}) \delta(r - (r_i^{a} - r_j^{a}))$$

and

$$G_R(r) = \sum_{i \neq j} |u_{ij}|^2 u_{ij}^2 - 2u_{ij}u_{ij}^2 Q_{ab} Q_{ab} \delta(r - (r_i^{a} - r_j^{a}))$$

with

$$u_{ij} \equiv \theta(\ell - |r_i^{a} - r_j^{a}|) .$$

These four-replica objects can be computed for any quadruplet of distinct replicas. The ensemble averaged correlation functions are simply obtained as $\Gamma_2 \equiv \Gamma_2/2$ and $G_R \equiv G_R/2$ and cf. the SI for a proof. We stress that one must keep the full space dependence of the correlators in the definitions above, as the introduction of shear breaks the rotational symmetry of the glass samples and so the correlators are not just functions of a distance $r$. 

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Numerics
To measure the quantities defined above, we performed molecular dynamics simulations of a Kob-Andersen 65-35% Lennard-Jones binary mixture in 2d. We have three system sizes, \( N = 1000, N = 4000 \) and \( N = 10000 \). We chose \( q_{12} \) with \( \ell = 0.3 \) in LJ units, but verified that changes in \( \ell \) leave the emerging picture invariant.

Following the procedure reported in Ref. (17), as a first step we prepared a glass by equilibrating the system at \( T = 0.4 \), and then quenching it (the rate is \( 10^{-6} \)) down to \( T = 1 \cdot 10^{-6} \) into a glassy configuration. The sample is then heated up again to \( T = 0.2 \), and a starting configuration of particle positions is chosen at this temperature. Note that while at \( T = 0.4 \) equilibration is sufficiently fast, at \( T = 0.2 \) the computation time is much shorter than the relaxation time. The configuration is then assigned a set of velocities randomly drawn from the Maxwell-Boltzmann distribution at \( T = 0.2 \), and these different samples are then quenched down to \( T = 0 \) at a rate of 0.1. This procedure can be repeated any number of times (say 100 times), and it allows us to get a sampling of the configurations, or replicas, inside one single “glassy patch”. We then perform this procedure again, using each time a different configuration from the parent melt at \( T = 0.4 \), and in doing so we get an ensemble of these glassy patches, each of them representing a distinct glass sample. For each of these patches, we measure the four- replica correlators defined above for any distinct quadruplet of replicas, averaging the result over any possible permutations of the quadruplet to gain statistics (29). The ensemble average is then performed by averaging the result over all the glass samples. To perform these measurement, below we use 100 patches for \( N = 1000 \), each with 100 configurations, 100 patches for \( N = 4000 \) each with 50 configurations and 50 patches for \( N = 10000 \) each with 50 configurations. A strain is then applied quasi-statically to all configurations in all patches. This creates an ensemble of strained patches for every value of the strain parameter \( \gamma \); from whence we measure again the above defined correlators, which then become functions of the strain \( \gamma \). This is simply a consequence of the response of the configurations, i.e. each position \( r \), in the definitions above becomes \( r \cdot \gamma \). Thus for example \( G_R(r) \) becomes \( G_R(r; \gamma) \) etc. We are interested in the behavior of the correlators as the yielding point \( \gamma_y \) is approached.

Results
We consider first the susceptibilities \( \chi_{GL}, \chi_{GR} \) and \( \chi_{G2} \) that can be obtained from the correlators, for example

\[
\chi_{GL}(\gamma) \equiv \int d^2 x \ G_L(x, y; \gamma)
\]

wherein yielding occurs. Since \( \chi_{GL} \) is much smaller in amplitude than \( \chi_{GR} \), there is no much new information in \( \chi_{GL} \) which is approximately \( 2 \chi_{GR} \).

More detailed information is provided by the full dependence of the correlators on their arguments. To see most clearly the change in the correlators as the spinodal point is approached, is best to consider for example the one-dimensional function \( G_R(x = 0, y; \gamma) \), shown for \( N = 4000 \) in Fig. 2. Similar results for the other systems sizes are available in the SI. We note that the correlator changes both in amplitude and in extent as we approach the critical point. To quantify these changes we fit a 3 parameter function to \( G_R(x = 0, y) \) in the form

\[
G_R(x = 0, y; \gamma) \approx C + A \exp(-y/\xi)
\]

where all the fitting coefficients are functions of \( \gamma \). In Fig. 3 we present the \( \gamma \) dependence of the amplitude \( A(\gamma) \), the constant \( C \) and the correlation length \( \xi(\gamma) \).

It is interesting to notice that the constant \( C \) decreases with the system size, presumably becoming irrelevant in the thermodynamic limit. The amplitude \( A \) is still increasing with the system size, and it is difficult to assert whether it converges or not. On the other hand we can safely conclude
that the data present a strong evidence for the increase in the correlation length; it is very likely that it should diverge in the thermodynamic limit.

Physical interpretation

To conclude this paper we present a physical interpretation to these new insights, connecting them to what is known about the mechanical yield in athermal amorphous solids. The most important characteristic of the mechanical yield in athermal amorphous solids is the change from plastic responses that are localized, typically in the form of Eshelby quadrupoles, to subextensive plastic events that are system spanning (31, 32). The energy drops associated with the localized Eshelby quadrupoles are system size independent, scaling like $N^\alpha$ where $N$ is the total number of particles in the system. Mechanical yield is associated with the spontaneous appearance of concatenated lines of quadrupoles (in 2 dimensions, or planes in 3 dimensions, (13, 15, 16)). The latter are associated with energy drops that are subextensive, scaling line $N^{1/3}$ in 2 dimensions. Importantly, the concatenated lines of quadrupoles change drastically the displacement field associated with the plastic events. Each quadrupole has an arm with a displacement field pointing outward and an arm with the displacement field pointing inward. When the quadrupole is isolated the displacement field decays algebraically to infinity. In contrast, when the quadrupoles are organized in the line there is a global connection between the outgoing direction of one quadrupole and the incoming direction of the next, making the displacement field strongly localized around the line of quadrupoles (or around a plane in 3 dimensions), and all the shear is there. This is a microscopic shear band. The main point of this paper is that the highly correlated phenomenon of such a shear band can only occur when there exists a correlation length that approaches the system size in magnitude. This is the correlation length $\xi$ that is identified in this paper, and cf. the upper panel of Fig. 3.

To understand the relevance of the spinodal point for this scenario, we provide two figures that were obtained in Ref. (17). In the upper panel of Fig. 4 one sees the order parameter $Q_{ab}$ as a function of $\gamma$, superimposed on the stress vs. strain curve of the system under study. The point “yield” was obtained with the help of the results shown in the lower panel, in which the probability of observing $Q_{ab}$ is plotted for values of $\gamma$ around the mechanical yield point $\gamma_y$. The yield itself is identified when the probability distribution function has two peaks of the same height. The spinodal point is at a slightly higher value of $\gamma$, where the peak occurring around high values of $Q_{ab}$ is about to disappear, with a characteris-

Fig. 2. The function $G_N(x = 0, y; \gamma)$ for various values of $\gamma$ from $5 \times 10^{-5}$ to 0.09405. Note the increase in the overall amplitude of the correlator as well as the increase in the correlation length. The lines through the data are the fit function Eq. (10).
the system is close to the spinodal, which, interestingly, is precisely the behavior of transient shear bands as reported in (21). In this thermal setting, we expect that the study of the ideas presented in this paper will have to proceed much as it does in the case of dynamical heterogeneities around the MCT crossover, entailing for example the definition and study of time-dependent multi-point susceptibilities and correlators.

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