Fracture and Second-Order Phase Transitions

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Using the global fiber bundle model as a tractable scheme of progressive fracture in heterogeneous materials, we define the branching ratio in avalanches as a suitable order parameter to clarify the order of the phase transition occurring at the collapse of the system. The model is analyzed using a probabilistic approach suited to smooth fluctuations. The branching ratio shows a behavior analogous to the magnetization in known magnetic systems with second-order phase transitions. We obtain a universal critical exponent $\beta \approx 0.5$ independent of the probability distribution used to assign the strengths of individual fibers.

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Interest in the fracture processes of heterogeneous media has increased in the last several years [1–4]. In the lab, a disordered material subjected to an increasing external load can be studied by measuring the acoustic emissions before the global rupture. It has been shown [5,6] that this intense precursory activity in the form of bursts of different microscopic sizes follows a well-defined power law. Despite the many efforts and successes that have been recently achieved, the question of whether rupture exhibits the properties of a first-order or a second-order phase transition remains under discussion, as well as what is the order parameter that indicates the type of transition.

From the theory side, the understanding of fracture in heterogeneous materials has progressed due to the use of lattice models and large scale simulations [3]. In this field, it is important to use models able to describe the complexity of the rupture process; nevertheless, they should be simple enough to permit analytical insight. To this class of models belong the well-known fiber bundle models (FBM) widely used since their introduction more than 40 years ago [7,8]. In static FBM, a set of fibers (elements) is located on a supporting lattice and one assigns to its elements a random strength threshold sampled from a probability distribution. The set is loaded and fibers break when their loads exceed their threshold values. In the equal load sharing (or global) FBM, which is the simplest scheme one can adopt to make the problem analytically tractable, one assumes that the load carried by failed elements is equally transferred. This implies that the load on any element is given by $\sigma = F/n_s(F)$, where $n_s$ is the number of surviving elements for a given $F$. The rupture of an element may induce secondary failures which in turn may trigger more failures, and so on. This process of induced failure at constant external load, termed an avalanche, stops when all surviving elements carry a load lower than their thresholds. The system is then loaded again and the process is repeated until the final catastrophic avalanche provokes the total rupture of the material, which occurs at a critical load $\sigma_c$ that depends on the probability distribution from where the individual strengths were drawn, as well as on the system size. The FBM have been recently used in self-organized criticality (SOC), a theoretical framework widely used for the study of avalanche phenomena in disordered systems. It has been shown using these models that systems with plastic behavior can reach a SOC state just before the global rupture [9]. A second case of self-organization with power law distributions in several quantities corresponds to the situation in which the fracture process coexists with a healing process [10].

In numerical simulations, the cycle of complete breakdown of the model is performed many times in order to average out the effect of fluctuations and obtain mean values. As we are interested in studying the behavior of the system as the critical point, or point of final collapse, is approached, it is of utmost importance to find a simple method able to capture the evolution of the system avoiding as much as possible the fluctuations appearing in numerical simulations. To introduce our probabilistic strategy, let there be a large set of $N_0$ elements. Suppose that each randomly from a probability distribution $P(\sigma)$. The system is then subjected to an external force $F$ such that each element increases its load in the same amount, $\sigma$. This individual stress (or load), $\sigma$, acts as the control parameter. The process of driving is done quasistatically; i.e., the external force is increased at a sufficiently slow rate as to produce a single breaking event when the stress on the weakest element equals its threshold value. Then, the increase of $F$ stops and the load of the broken element is equally transferred. This implies that the load on any element is given by $\sigma = F/n_s(F)$, where $n_s$ is the number of surviving elements for a given $F$. The rupture of an element may induce secondary failures which in turn may trigger more failures, and so on. This process of induced failure at constant external load, termed an avalanche, stops when all surviving elements carry a load lower than their thresholds. The system is then loaded again and the process is repeated until the final catastrophic avalanche provokes the total rupture of the material, which occurs at a critical load $\sigma_c$ that depends on the probability distribution from where the individual strengths were drawn, as well as on the system size. The FBM have been recently used in self-organized criticality (SOC), a theoretical framework widely used for the study of avalanche phenomena in disordered systems. It has been shown using these models that systems with plastic behavior can reach a SOC state just before the global rupture [9]. A second case of self-organization with power law distributions in several quantities corresponds to the situation in which the fracture process coexists with a healing process [10].

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element carries a given load $\sigma$, which is zero at the initial state. The strength of each element is drawn from a probability distribution $P(\sigma)$. Different probability distributions can be considered. In materials science the Weibull distribution is widely used,

$$P(\sigma) = 1 - e^{-\left(\frac{\sigma}{\sigma_0}\right)^\rho}, \quad (1)$$

where $\rho$ is the so-called Weibull index, which controls the degree of disorder in the system (the bigger the Weibull index, the smaller the disorder), and $\sigma_0$ is a load of reference. In the following we assume $\sigma_0 = 1$, and therefore the loads are dimensionless. At this point, it is worth noting that the results and the formulas derived in the following hold for a wide class of probability distributions. We use here the Weibull distribution for definiteness, but results have also been obtained for other distributions.

Equation (1) represents the probability that an element fails under the individual load $\sigma$. Now, consider the case in which an element drawn from Eq. (1) supports a load $\sigma_1$ but breaks under a new load $\sigma_2$. The probability that this happens is given by

$$p(\sigma_1, \sigma_2) = \frac{P(\sigma_2) - P(\sigma_1)}{1 - P(\sigma_1)} = 1 - e^{-\left(\sigma_2^{-1} - \sigma_1^{-1}\right)} \quad (2)$$

So, the probability $q(\sigma_1, \sigma_2)$ that an element that has survived to the load $\sigma_1$ also survives to the load $\sigma_2$ will be given by $q(\sigma_1, \sigma_2) = 1 - p(\sigma_1, \sigma_2) = e^{-\left(\sigma_2^{-1} - \sigma_1^{-1}\right)}$.

To mimic the quasistatic increase in load on the system we impose the condition that under an external force $F$, the next breaking event consists of one single failure. Let us suppose that after the latest avalanche, there are $N_k$ surviving elements, each one bearing a load $\sigma_k$. The new individual load $\sigma_1$ needed to provoke the failure of just one more element is given by the solution of $N_k - 1 = N_k q(\sigma_k, \sigma_1)$. Thus,

$$\sigma_1 = \left[\sigma_k^\rho - \ln\left(1 - \frac{1}{N_k}\right)\right]^{1/\rho}, \quad (3)$$

where in Eq. (3) $N_k = N_0$ and $\sigma_2 = 0$ at the initial state. Elevating the external force up to the $N_k \sigma_1$ level, statistically speaking, one element breaks. As we are dealing with an equal load sharing set, the choice of the broken element is irrelevant because all the elements are equivalent. Once the first element fails, the redistribution of its stress takes place. This may induce other failures until the end of the avalanche.

Now, how many elements will survive to the situation in which $n_1$ elements with load $\sigma_1$ fail in an avalanche step? The new load on the intact $N_1 - n_1 = N_2$ elements is $\sigma_2 = N_1 \sigma_1 / N_2$. So, the number $N_3$ of elements that survive to the new load can be expressed as

$$N_3 = N_2 q\left(\sigma_1, \frac{N_1}{N_2} \sigma_1\right) = N_2 q(\sigma_1, \sigma_2). \quad (4)$$

As a consequence of applying Eq. (4), $N_2 - N_3$ elements break and the new total number of intact fibers will support a bigger load $\sigma_3$. The avalanche may continue and Eq. (4) is applied again for the set of $N_3$ surviving elements. The iterative process will stop when no new element fails, which occurs when the right-hand side is equal to the left-hand side in Eq. (4). The general form of Eq. (4) is

$$N_{j+1} = N_j q(\sigma_{j-1}, \sigma_j), \quad (5)$$

with the conservation condition for the total load in the system during an avalanche

$$N_j \sigma_j = N_{j-1} \sigma_{j-1} \quad (6)$$

and the condition

$$N_j = N_{j+1}, \quad (7)$$

which determines the end of the avalanche. The dynamics of the system is determined by Eqs. (3), (5), and (6). The size of an avalanche is given by the number of elements that break between two successive steps of external loading. The critical load, defined as the load needed to provoke the total collapse of the system, is equal to the load on the intact elements just before the final catastrophic avalanche. Note that in this probabilistic approach, in contrast to Monte Carlo simulations, we need to store only the information concerning the loads on the intact elements; that is, the details of the threshold list are omitted.

In the probabilistic strategy, we can proceed in two different ways in order to determine when an avalanche ends, which we refer to as the continuous and discrete cases. For the continuous case, the number $N_{j+1}$ of surviving elements is considered a real number. Strictly speaking, this means that condition (7) is never fulfilled. So, condition (7) is replaced in numerical calculations by using a factor $\nu \ll 1$ that determines the end of an avalanche, i.e., if $N_j - N_{j+1} \leq \nu$ the avalanche stops; otherwise it continues. In the discrete case, $N_{j+1}$ is considered to be a whole number, so that after each iteration of Eq. (5), $N_{j+1}$ has to be rounded up. This is done comparing the remainder of $N_{j+1}$, $\lambda$, with a random number $\alpha$ uniformly distributed in the interval $[0,1]$. Thus, if $\alpha \geq \lambda$, $N_{j+1}$ is equal to its whole part, otherwise, $N_{j+1}$ is equal to its whole part plus one. Next, we check whether the condition (7) is satisfied for the rounded value of $N_{j+1}$ or if a new iteration of Eq. (5) has to be performed. The continuous approach has the advantage that the fluctuations are ruled out, whereas for the discrete case the results are similar to those obtained by Monte Carlo simulations where it is necessary to average over many realizations in order to get accurate mean values. Remember that in this model the central limit theorem applies [11].

In Fig. 1 we have depicted the fraction of broken elements versus $\sigma$, for the continuous case and for four individual Monte Carlo simulations with a Weibull index $\rho = 2$ and $N_0 = 5000$. No averaging has been done because our aim is only to illustrate the scatter of the results. As can be seen, the continuous probabilistic model
FIG. 1. Fraction of broken elements for the equal load sharing model. The line corresponds to the results obtained with the continuous approach and gray dots correspond to four Monte Carlo realizations.

gives a smooth curve and provides an accurate value for the critical load \( \sigma_c \), which analytically is given by

\[
\sigma_c = (\rho e)^{-1/\rho}
\]

in the limit of infinite \( N_0 \).

Now, we proceed to explore the behavior of some quantities as the critical point is reached. The results shown below have been obtained using the continuous approach (\( \rho = 2 \)). In Fig. 2 we show the interesting scaling relation for the average avalanche size. It turns out that the avalanche size near to the critical point diverges with an exponent \( \gamma = \frac{1}{2} \) as

\[
s \sim (\sigma_c - \sigma)^{-\gamma}.
\]

A similar behavior, through a mapping of a fuse network model to the global fiber bundle model used here, has recently been reported [2]. We have also obtained the same scaling function for the derivative of the number of broken fibers with respect to the load on the system. The rate \( dN/d\sigma \) diverges as

\[
(\sigma_c - \sigma)^{-1/2},
\]

thus qualifying a critical mean field behavior as was already shown in Ref. [4]. In Ref. [9], a similar scaling behavior is addressed for the derivative of the strain carried by the fibers with respect to the driving force.

Another way to shed light on the critical behavior of this type of system is to define a branching ratio \( \zeta \) for each avalanche. This magnitude represents the probability to trigger future breaking events given an initial individual failure [12,13] and is related to the number of broken fibers by

\[
\zeta = \frac{\langle z \rangle - 1}{\langle z \rangle}.
\]  

The above relation can be obtained by thinking of the evolution of fracture as a kind of branching process [14]. In this process, each node gives rise to a number \( n \) of new branches in the next time step. The average number \( \langle n \rangle \) of new branches is called the branching ratio. Let us denote by \( n_t \) the number of branches at a given step \( t \) of the branching process, and by \( t_{\text{max}} \) the total number of time steps before it dies. Then,

\[
\zeta = 1 - \frac{n_0}{\sum_{t=0}^{t_{\text{max}}} n_t}.
\]

As, \( n_0 = 1 \), \( \zeta = 1 - \frac{1}{n_{\text{tot}}} \), where \( n_{\text{tot}} \) is the total number of nodes developed in the branching process. For a fracture process, \( n_{\text{tot}} \) is equal to the average number of failure events. So, Eq. (8) defines the branching ratio. We represent by \( \langle z \rangle \) the average number of elements that fail in one avalanche, which is a function of \( \sigma \) and coincides with \( s \).

This analogy between fracture and branching processes has been previously used to study the criticality in the process of fragmentation of Hg drops [15]. The branching ratio will then act as the order parameter. It takes the value 1 when the system is critical thereby representing a measure of the distance of the system from the critical state [13]. We have numerically computed \( \zeta \) by means of the continuous method. The results obtained for a system of \( N_0 = 50000 \) elements and several values of \( \rho \) have been plotted in Fig. 3. It can be seen in this figure that \( 1 - \zeta \)
numerical results also fit the mean-field result for avalanche sizes, which also diverge at that point. Our fiber failures as the critical point is reached, and for the have obtained the same scaling relation for the rate of breakdown and fracture, the authors present numerical and instability [16]. There, by simulating models of electric collapse of the system. The result that at $\sigma_c \zeta \to 1$ is consistent with the previous result that the avalanche size diverges at the critical point. On the other hand, the branching ratio does not depend on the size of the system for large systems, in contrast with previous results in other fracturing systems [13].

The suggestion of Ref. [2] is that fracture can be seen as a first-order phase transition close to a spinodal-like instability [16]. There, by simulating models of electric breakdown and fracture, the authors present numerical and theoretical evidence of several scaling relations and of a discrete jump in some macroscopic properties. Here, we have obtained the same scaling relation for the rate of fiber failures as the critical point is reached, and for the avalanche sizes, which also diverge at that point. Our numerical results also fit the mean-field result $\gamma = \frac{1}{2}$. It is true that the fraction of unbroken fibers just before the global rupture has a discontinuity, but from our point of view, that is not enough to set the conclusion that fracture can be described as a first-order phase transition, since the concepts related to spinodal nucleation are not sufficiently well established in driven disordered systems.

Our alternative point of view has been to consider the branching ratio as an appropriate order parameter. According to the results obtained, the branching ratio goes continuously from zero to one. Note, additionally, that what changes discontinuously at $\sigma_c$ is the rate of change of $\xi$ rather than $\xi$ itself, which is, in essence, a continuous phase change. Therefore, the behavior of the branching ratio implies that the system undergoes a second-order phase transition as claimed in another analysis of fracture models [17]. Our results suggest that fracture in heterogeneous systems with long-range interaction can be described as a phase transition of the second-order type. Besides, it is important to bear in mind that in fiber models with local interactions, the order parameter $\xi$ has a discontinuous jump typical of first-order phase transitions. Finally, it is worth recalling that fracture of real materials is a process based on elasticity, and elasticity is a long-range phenomenon. In this respect, the global load-sharing model we have explored here could be a better analogy to real fracture than the local one.

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